

# Structured Data: Dependency, Testing (Kernel, RKHS)

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∈ Structured Data: Learning, Prediction, **Dependency**, **Testing**  
M2 Data Science, University of Paris-Saclay

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- 1 Concepts from **functional analysis**:
  - normed-, inner product space,
  - convergent-, Cauchy sequence,
  - complete spaces: Banach-, Hilbert space,
  - continuous/bounded linear operators.

## ② RKHS:

- different views:
  - ① continuous evaluation functional,
  - ② reproducing kernel,
  - ③ positive definite function,
  - ④ feature view (kernel).
- equivalence, explicit construction.

We define the 'length' of a vector.

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Note:

- norm  $\Rightarrow$  metric:  $d(f, g) = \|f - g\| \Rightarrow$
- study **continuity**, **convergence**.

- $(\mathbb{R}, |\cdot|)$ ,
- $(\mathbb{R}^d, \|\mathbf{x}\|_p = [\sum_i |x_i|^p]^{\frac{1}{p}})$ ,  $1 \leq p$ .
  - $p = 1$ :  $\|\mathbf{x}\|_1 = \sum_i |x_i|$  (Manhattan),
  - $p = 2$ :  $\|\mathbf{x}\|_2 = \sqrt{\sum_i x_i^2}$  (Euclidean),
  - $p = \infty$ :  $\|\mathbf{x}\|_\infty = \max_i |x_i|$  (maximum norm).
- $(C[a, b], \|f\|_p = [\int_a^b |f(x)|^p dx]^{\frac{1}{p}})$ ,  $1 \leq p$ .



$\mathcal{F}$ : vector space over  $\mathbb{R}$ .  $\langle \cdot, \cdot \rangle : \mathcal{F} \times \mathcal{F} \rightarrow \mathbb{R}$  is an **inner product** on  $\mathcal{F}$  if for  $\forall \alpha_j \in \mathbb{R}, f_i, f, g \in \mathcal{F}$

①  $\langle \alpha_1 f_1 + \alpha_2 f_2, g \rangle = \alpha_1 \langle f_1, g \rangle + \alpha_2 \langle f_2, g \rangle$  (linearity),

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Notes:

- 1, 2  $\Rightarrow$  bilinearity.
- inner product  $\Rightarrow$  norm:  $\|f\| = \sqrt{\langle f, f \rangle}$ .
- 1,2,3' ( $\langle f, f \rangle \geq 0$ ) is called **semi-inner product**.

- $(\mathbb{R}^d, \langle \mathbf{x}, \mathbf{y} \rangle = \sum_i x_i y_i)$ .
- $(\mathbb{R}^{d_1 \times d_2}, \langle \mathbf{A}, \mathbf{B} \rangle_F = \text{tr}(\mathbf{A}^T \mathbf{B}) = \sum_{ij} A_{ij} B_{ij})$ .
- $(C[a, b], \langle f, g \rangle = \int_a^b f(x)g(x)dx)$ .

Relations:

- $|\langle f, g \rangle| \leq \|f\| \cdot \|g\|$  (CBS),
- $4 \langle f, g \rangle = \|f + g\|^2 - \|f - g\|^2$  (polarization identity),
- $\|f + g\|^2 + \|f - g\|^2 = 2 \|f\|^2 + 2 \|g\|^2$  (parallelogram law).

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Notes:

- CBS holds for semi-inner products.
- parallelogram law = characterization of ' $\|\cdot\| \leftarrow \langle \cdot, \cdot \rangle$ '.

# Convergent-, Cauchy sequence

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- **Convergent sequence:**  $f_n \xrightarrow{\mathcal{F}} f$  if  $\forall \epsilon > 0 \exists N = N(\epsilon) \in \mathbb{N}$ , s.t.  
 $\forall n \geq N, \|f_n - f\|_{\mathcal{F}} < \epsilon$ .



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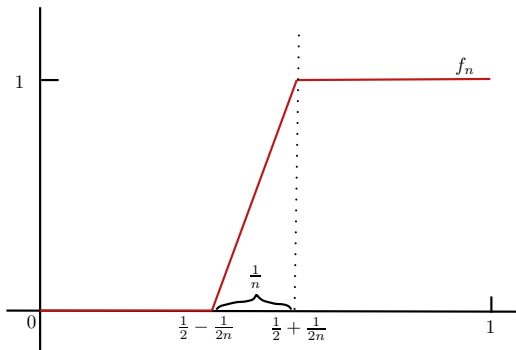
Note:

- **convergent  $\Rightarrow$  Cauchy:**  $\|f_n - f_m\|_{\mathcal{F}} \leq \|f_n - f\|_{\mathcal{F}} + \|f - f_m\|_{\mathcal{F}}$ .

# Not every Cauchy sequence converges

Examples:

- $1, 1.4, 1.41, 1.414, 1.4142, \dots$ : Cauchy in  $\mathbb{Q}$ , but  $\sqrt{2} \notin \mathbb{Q}$ .
- $(C[0, 1], \|\cdot\|_{L^2[0,1]})$ :



But a Cauchy sequence is bounded.

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- **Banach space** = complete normed space, e.g.

① Let  $p \in [1, \infty)$ ,  $L^p(\mathcal{X}, \mathcal{A}, \mu) :=$

$$\left\{ f : (\mathcal{X}, \mathcal{A}) \rightarrow \mathbb{R} \text{ measurable} : \|f\|_p = \left[ \int_{\mathcal{X}} |f(x)|^p d\mu(x) \right]^{1/p} < \infty \right\}.$$

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- **Hilbert space** = complete inner product space;  $L^2(\mathcal{X}, \mathcal{A}, \mu)$ .

# Linear-, bounded operator

$\mathcal{F}, \mathcal{G}$ : normed spaces.  $A : \mathcal{F} \rightarrow \mathcal{G}$  is called

- **linear operator**:

- ①  $A(\alpha f) = \alpha (Af) \quad \forall \alpha \in \mathbb{R}, f \in \mathcal{F}$ , (homogeneity),

- ②  $A(f + g) = Af + Ag \quad \forall f, g \in \mathcal{F}$  (additivity).

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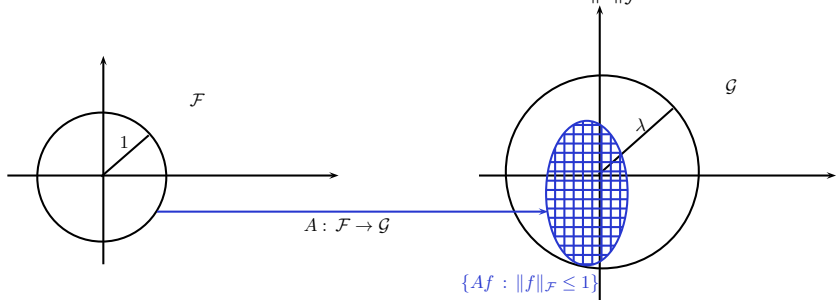
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$\mathcal{G} = \mathbb{R}$ : **linear functional**.

- **bounded operator**:  $A$  is linear &  $\|A\| = \sup_{f \in \mathcal{F}} \frac{\|Af\|_{\mathcal{G}}}{\|f\|_{\mathcal{F}}} < \infty$ .





# Unbounded linear functional: example

$(C^1[0, 1], \|f\|_\infty := \max_{x \in [0, 1]} |f(x)|)$ ,  $A(f) = f'(0) \in \mathbb{R}$ :

- 1  $A$ : linear  $\Leftarrow$  differentiation & evaluation are linear,
- 2  $f_n(x) = e^{-nx}$  ( $n \in \mathbb{Z}^+$ ):
  - $\|f_n\|_\infty \leq 1$ , but
  - $|A(f_n)| = |f'_n(0)| = \left| -ne^{-nx} \Big|_{x=0} \right| = |-n| = n \rightarrow \infty$ .

- Def.:  $A$  is

- **continuous at**  $f_0 \in \mathcal{F}$ :  $\forall \epsilon > 0 \exists \delta = \delta(\epsilon, f_0) > 0$ , s.t.

$$\|f - f_0\|_{\mathcal{F}} < \delta \quad \text{implies} \quad \|Af - Af_0\|_{\mathcal{G}} < \epsilon.$$

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- Example:

- Let  $A_g(f) := \langle f, g \rangle_{\mathcal{F}} \in \mathbb{R}$ , where  $f, g \in \mathcal{F}$ .
- $A_g$  is Lipschitz continuous:

$$|A_g(f_1) - A_g(f_2)| \stackrel{\langle \cdot, \cdot \rangle_{\mathcal{F}}: \text{lin.}}{=} |\langle f_1 - f_2, g \rangle_{\mathcal{F}}| \stackrel{\text{CBS}}{\leq} \|g\|_{\mathcal{F}} \|f_1 - f_2\|_{\mathcal{F}}.$$

Theorem:

- $A$ : **linear** operator. Equivalent:  $A$  is
  - 1 continuous,
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  - 3 bounded.

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- $A$ : **linear** operator. Equivalent:  $A$  is
  - 1 continuous,
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  - 3 bounded.
- Riesz representation ( $\mathcal{F}$ : Hilbert,  $\mathcal{G} = \mathbb{R}$ ):

$$\text{continuous linear functionals} = \{ \langle \cdot, g \rangle_{\mathcal{F}} : g \in \mathcal{F} \}.$$

Let us switch to RKHS-s!

$$k_G(a, b) = e^{-\frac{\|a-b\|_2^2}{2\theta^2}}, \quad k_e(a, b) = e^{-\frac{\|a-b\|_2}{2\theta^2}},$$

$$k_C(a, b) = \frac{1}{1 + \frac{\|a-b\|_2^2}{\theta^2}}, \quad k_t(a, b) = \frac{1}{1 + \|a-b\|_2^\theta},$$

$$k_p(a, b) = (\langle a, b \rangle + \theta)^p, \quad k_r(a, b) = 1 - \frac{\|a-b\|_2^2}{\|a-b\|_2^2 + \theta},$$

$$k_i(a, b) = \frac{1}{\sqrt{\|a-b\|_2^2 + \theta^2}},$$

$$k_{M, \frac{3}{2}}(a, b) = \left(1 + \frac{\sqrt{3} \|a-b\|_2}{\theta}\right) e^{-\frac{\sqrt{3} \|a-b\|_2}{\theta}},$$

$$k_{M, \frac{5}{2}}(a, b) = \left(1 + \frac{\sqrt{5} \|a-b\|_2}{\theta} + \frac{5 \|a-b\|_2^2}{3\theta^2}\right) e^{-\frac{\sqrt{5} \|a-b\|_2}{\theta}}.$$

## View-1: continuous evaluation.

- Let  $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$  be a Hilbert space.
- Consider for fixed  $x \in \mathcal{X}$  the  $\delta_x : f \in \mathcal{H} \mapsto f(x) \in \mathbb{R}$  map.



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- The (Dirac) evaluation functional is **linear**:

$$\begin{aligned}\delta_x(\alpha f + \beta g) &= (\alpha f + \beta g)(x) = \alpha f(x) + \beta g(x) \\ &= \alpha \delta_x(f) + \beta \delta_x(g) \quad (\forall \alpha, \beta \in \mathbb{R}, f, g \in \mathcal{H}).\end{aligned}$$

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- Def.:  $\mathcal{H}$  is called **RKHS** if  $\delta_x$  is **continuous**  $\forall x \in \mathcal{X}$ .

## Example for non-continuous $\delta_x$

$\mathcal{H} = L^2[0, 1] \ni f_n(x) = x^n$ :

①  $f_n \rightarrow 0 \in \mathcal{H}$  since

$$\lim_{n \rightarrow \infty} \|f_n - 0\|_2 = \lim_{n \rightarrow \infty} \left( \int_0^1 x^{2n} dx \right)^{1/2} = \lim_{n \rightarrow \infty} \frac{1}{\sqrt{2n+1}} = 0,$$

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② but  $\delta_1(f_n) = 1 \not\rightarrow \delta_1(0) = 0$ .

In  $L^2$ : norm convergence  $\not\Rightarrow$  pointwise convergence.

In RKHS: convergence in norm  $\Rightarrow$  pointwise convergence!

- Result:  $f_n \xrightarrow{\mathcal{H}} f \Rightarrow f_n \xrightarrow{\forall x} f$ .

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- Result:  $f_n \xrightarrow{\mathcal{H}} f \Rightarrow f_n \xrightarrow{\forall x} f$ .
- Proof: For any  $x \in \mathcal{X}$ ,

$$\begin{aligned} |f_n(x) - f(x)| &\stackrel{\delta_x \text{ def}}{=} |\delta_x(f_n) - \delta_x(f)| \stackrel{\delta_x \text{ lin}}{=} |\delta_x(f_n - f)| \\ &\stackrel{\delta_x: \text{ bounded}}{\leq} \underbrace{\|\delta_x\|}_{< \infty} \underbrace{\|f_n - f\|_{\mathcal{H}}}_{\rightarrow 0}. \end{aligned}$$

View-2: reproducing  $\Rightarrow$  elements, kernel trick.

- Let  $\mathcal{H}$  be a Hilbert space of  $\mathcal{X} \rightarrow \mathbb{R}$  functions.
- $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  is called a **reproducing kernel of  $\mathcal{H}$**  if for  $\forall x \in \mathcal{X}$ 
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## Questions

Uniqueness, existence?

Reproducibility & norm definition  $\Rightarrow$  uniqueness.

- Let  $k_1, k_2$  be r.k.-s of  $\mathcal{H}$ . Then for  $\forall f \in \mathcal{H}, \forall x \in \mathcal{X}$

$$\langle f, k_1(\cdot, x) - k_2(\cdot, x) \rangle_{\mathcal{H}} \stackrel{\langle \cdot, \cdot \rangle_{\mathcal{H}} \text{ lin, } k_i \text{ r.k.}}{=} f(x) - f(x) = 0.$$

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- Choosing  $f = k_1(\cdot, x) - k_2(\cdot, x)$ , we get

$$\|k_1(\cdot, x) - k_2(\cdot, x)\|_{\mathcal{H}}^2 = 0, \quad (\forall x \in \mathcal{X})$$

i.e.,  $k_1 = k_2$ .

- Result:  $\mathcal{H}$  has a r.k. ( $k$ )  $\Leftrightarrow \mathcal{H}$  is a RKHS.

## View-2 (r.k.) $\Leftrightarrow$ view-1 (RKHS)

- Result:  $\mathcal{H}$  has a r.k.  $(k) \Leftrightarrow \mathcal{H}$  is a RKHS.
- Proof ( $\Rightarrow$ ):

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i.e.  $\delta_x : \mathcal{H} \rightarrow \mathbb{R}$  is bounded (hence continuous).

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Convergence in RKHS  $\Rightarrow$  **uniform** convergence! ( $k$ : bounded).

# View-2 (r.k.) $\Leftrightarrow$ view-1 (RKHS): $\Leftarrow$ , existence of r.k.

Proof ( $\Leftarrow$ ): Let  $\delta_x$  be continuous for all  $x \in \mathcal{X}$ .

① By the Riesz repr. theorem  $\exists f_{\delta_x} \in \mathcal{H}$

$$\delta_x(f) = \langle f, \underbrace{f_{\delta_x}}_{=k(\cdot, x)?} \rangle_{\mathcal{H}}, \forall f \in \mathcal{H}.$$

# View-2 (r.k.) $\Leftrightarrow$ view-1 (RKHS): $\Leftarrow$ , existence of r.k.

Proof ( $\Leftarrow$ ): Let  $\delta_x$  be continuous for all  $x \in \mathcal{X}$ .

- ① By the Riesz repr. theorem  $\exists f_{\delta_x} \in \mathcal{H}$

$$\delta_x(f) = \langle f, \underbrace{f_{\delta_x}}_{=k(\cdot, x)?} \rangle_{\mathcal{H}}, \forall f \in \mathcal{H}.$$

- ② Let  $k(x', x) = f_{\delta_x}(x')$ ,  $\forall x, x' \in \mathcal{X}$ , then

$$k(\cdot, x) = f_{\delta_x} \in \mathcal{H},$$
$$\langle f, k(\cdot, x) \rangle_{\mathcal{H}} = \delta_x(f) = f(x).$$

Thus,  $k$  is the reproducing kernel.

### View-3: positive definiteness.

- Let  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  be a symmetric function.

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- $\mathbf{G} := [k(x_i, x_j)]_{i,j=1}^n$ : Gram matrix.
- $k$  is called **positive definite**, if

$$\mathbf{a}^T \mathbf{G} \mathbf{a} \geq 0$$

for  $\forall n \geq 1, \forall \mathbf{a} \in \mathbb{R}^n, \forall (x_1, \dots, x_n) \in \mathcal{X}^n$ .

#### View-4: 'kernel as inner product' view.

- Def.: A  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  function is called **kernel**, if
  - 1  $\exists \phi : \mathcal{X} \rightarrow \mathcal{F}$ , where  $\mathcal{F}$  is a Hilbert space s.t.
  - 2  $k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{F}}$ .
- Intuition:  $k$  is **inner product** in  $\mathcal{F}$ .

- Every r.k. is a kernel:  $\phi(x) := k(\cdot, x)$ ,  $k(x, y) = \langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}}$ .
- Every kernel is positive definite:

$$\mathbf{a}^T \mathbf{G} \mathbf{a} = \sum_{i=1}^n \sum_{j=1}^n a_i a_j k(x_i, x_j)$$

$$\stackrel{k \text{ def}}{=} \underset{\langle \cdot, \cdot \rangle_{\mathcal{F}} \text{ lin}}{\left\langle \sum_{i=1}^n a_i \phi(x_i), \sum_{j=1}^n a_j \phi(x_j) \right\rangle_{\mathcal{F}}}$$

$$\stackrel{\|\cdot\|_{\mathcal{F}} = \sqrt{\langle \cdot, \cdot \rangle_{\mathcal{F}}}}{=} \left\| \sum_{i=1}^n a_i \phi(x_i) \right\|_{\mathcal{F}}^2 \geq 0.$$



- Result-1 (proved):  
RKHS ( $\delta_x$  continuous)  $\Leftrightarrow$  reproducing kernel.
- Result-2 (proved):  
reproducing kernel  $\Rightarrow$  kernel  $\Rightarrow$  positive definite.

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Moore-Aronszajn theorem (follows)

positive definite  $\Rightarrow$  reproducing kernel.

$\Rightarrow$  the 4 notions are *exactly* the same!

# Moore-Aronszajn construction: high-level view

- Given: a  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  positive definite function.
- We construct a pre-RKHS  $\mathcal{H}_0$ :

$$\mathcal{H}_0 = \left\{ f = \sum_{i=1}^n \alpha_i k(\cdot, x_i) : \alpha_i \in \mathbb{R}, x_i \in \mathcal{X} \right\} \supseteq \{k(\cdot, x) : x \in \mathcal{X}\},$$

$$\langle f, g \rangle_{\mathcal{H}_0} = k(x, y),$$

where  $f = k(\cdot, x)$ ,  $g = k(\cdot, y)$ .

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$$\langle f, g \rangle_{\mathcal{H}_0} = \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j k(x_i, y_j),$$

where  $f = \sum_{i=1}^n \alpha_i k(\cdot, x_i)$ ,  $g = \sum_{j=1}^m \beta_j k(\cdot, y_j)$ .

- $\mathcal{H}_0$  will satisfy:
  - 0 linear space ( $\checkmark$ );  $\langle f, g \rangle_{\mathcal{H}_0}$ : well-defined & inner product.
  - 1  $\delta_x$ -s are continuous on  $\mathcal{H}_0$  ( $\forall x$ ).
  - 2 For any  $\{f_n\} \subset \mathcal{H}_0$  Cauchy seq.:

$$f_n \xrightarrow{\forall x} 0 \quad \Rightarrow \quad f_n \xrightarrow{\mathcal{H}_0} 0.$$

- From  $\mathcal{H}_0$  we construct  $\mathcal{H}$  as:
  - 1  $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ , for which
  - 2  $\exists \{f_n\}$   $\mathcal{H}_0$ -Cauchy seq. such that  $f_n \xrightarrow{\forall x} f$ .

- Let

$$\langle f, g \rangle_{\mathcal{H}} := \lim_{n \rightarrow \infty} \langle f_n, g_n \rangle_{\mathcal{H}_0}, \quad (1)$$

where  $f_n \xrightarrow{\forall x} f$ ,  $g_n \xrightarrow{\forall x} g$   $\mathcal{H}_0$ -Cauchy sequences.

- $\mathcal{H}$  will satisfy:

- $\mathcal{H}_0 \subset \mathcal{H}$ :  $\checkmark [f_n \equiv f \in \mathcal{H}_0]$ .
- $\mathcal{H}$  is a RKHS with r.k.  $k$ :
  - 1  $\mathcal{H}$ : linear space ( $\checkmark$ ),
  - 0  $\langle f, g \rangle_{\mathcal{H}}$ : well-defined & inner product.
  - 1  $\mathcal{H}$  is complete.
  - 2  $\delta_x$ -s are continuous on  $\mathcal{H}$  ( $\forall x$ ).
  - 3  $\mathcal{H}$  has r.k.  $k$  (used to define  $\mathcal{H}_0$ ).

$\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$ : well-defined,  $k$  reproducing on  $\mathcal{H}_0$

- Recall: if  $f = \sum_{i=1}^n \alpha_i k(\cdot, x_i)$ ,  $g = \sum_{j=1}^m \beta_j k(\cdot, y_j)$ , then

$$\langle f, g \rangle_{\mathcal{H}_0} = \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j k(x_i, y_j).$$

- $\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$  is independent of the particular  $\{\alpha_i\}$  and  $\{\beta_j\}$ :

$$\langle f, g \rangle_{\mathcal{H}_0} = \sum_{i=1}^n \alpha_i \sum_{j=1}^m \beta_j k(x_i, y_j) = \sum_{i=1}^n \alpha_i g(x_i) \left[ = \sum_{j=1}^m \beta_j f(y_j) \right].$$



## $\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$ : well-defined, $k$ reproducing on $\mathcal{H}_0$

- Recall: if  $f = \sum_{i=1}^n \alpha_i k(\cdot, x_i)$ ,  $g = \sum_{j=1}^m \beta_j k(\cdot, y_j)$ , then

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- $\Rightarrow$  reproducing property on  $\mathcal{H}_0$ :

$$\langle f, k(\cdot, x) \rangle_{\mathcal{H}_0} = \sum_{i=1}^n \alpha_i k(x_i, x) = f(x).$$

- The 'tricky' property to check:

$$\|f\|_{\mathcal{H}_0} := \langle f, f \rangle_{\mathcal{H}_0} = 0 \implies f = 0.$$

- This holds by CBS (for the semi-inner product  $\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$ ):  $\forall x$

$$|f(x)| \stackrel{\text{k r.k. on } \mathcal{H}_0}{=} |\langle f, k(\cdot, x) \rangle_{\mathcal{H}_0}| \stackrel{\text{CBS}}{\leq} \underbrace{\|f\|_{\mathcal{H}_0}}_{=0} \sqrt{k(x, x)} = 0.$$

$\delta_x$  is continuous on  $\mathcal{H}_0$  ( $\forall x$ ): Let  $f, g \in \mathcal{H}_0$ , then

$$\begin{aligned} |\delta_x(f) - \delta_x(g)| &\stackrel{\delta_x \text{ def, } k \text{ r.k., } \langle \cdot, \cdot \rangle_{\mathcal{H}_0} \text{ lin}}{=} |\langle f - g, k(\cdot, x) \rangle_{\mathcal{H}_0}| \\ &\stackrel{\text{CBS, } k \text{ r.k.}}{\leq} \sqrt{k(x, x)} \|f - g\|_{\mathcal{H}_0}. \end{aligned}$$

$f_n : \mathcal{H}_0$ -Cauchy  $\xrightarrow{(\forall x)} 0 \Rightarrow f_n \xrightarrow{\mathcal{H}_0} 0$ :

- $f_n$ : Cauchy  $\Rightarrow$  bounded, i.e.  $\|f_n\|_{\mathcal{H}_0} < A$ .
- $f_n$ : Cauchy  $\Rightarrow n, m \geq \exists N_1: \|f_n - f_m\|_{\mathcal{H}_0} < \epsilon/(2A)$ .
- Let  $f_{N_1} = \sum_{i=1}^r \alpha_i k(\cdot, x_i)$ .  $n \geq \exists N_2: |f_n(x_i)| < \frac{\epsilon}{2r|\alpha_i|}$  ( $i = 1, \dots, r$ ).

For  $n \geq \max(N_1, N_2)$ :

$$\|f_n\|_{\mathcal{H}_0}^2 < \epsilon.$$

## Pre-RKHS: main property-2

$f_n : \mathcal{H}_0$ -Cauchy  $\xrightarrow{(\forall x)} 0 \Rightarrow f_n \xrightarrow{\mathcal{H}_0} 0$ :

- $f_n$ : Cauchy  $\Rightarrow$  bounded, i.e.  $\|f_n\|_{\mathcal{H}_0} < A$ .
- $f_n$ : Cauchy  $\Rightarrow n, m \geq \exists N_1: \|f_n - f_m\|_{\mathcal{H}_0} < \epsilon/(2A)$ .
- Let  $f_{N_1} = \sum_{i=1}^r \alpha_i k(\cdot, x_i)$ .  $n \geq \exists N_2: |f_n(x_i)| < \frac{\epsilon}{2r|\alpha_i|}$  ( $i = 1, \dots, r$ ).

For  $n \geq \max(N_1, N_2)$ :

$$\begin{aligned} \|f_n\|_{\mathcal{H}_0}^2 &= \langle f_n, f_n \rangle_{\mathcal{H}_0} \leq |\langle f_n - f_{N_1}, f_n \rangle_{\mathcal{H}_0}| + |\langle f_{N_1}, f_n \rangle_{\mathcal{H}_0}| \\ &\leq \underbrace{\|f_n - f_{N_1}\|_{\mathcal{H}_0} \|f_n\|_{\mathcal{H}_0}}_{< [\epsilon/(2A)]A = \frac{\epsilon}{2}} + \sum_{i=1}^r \underbrace{|\alpha_i f_n(x_i)|}_{< |\alpha_i| \frac{\epsilon}{2r|\alpha_i|}} < \epsilon. \end{aligned}$$

$\langle \cdot, \cdot \rangle_{\mathcal{H}}$ : well-defined

$\alpha_n = \langle f_n, g_n \rangle_{\mathcal{H}_0}$  is convergent by Cauchy'sness in  $\mathbb{R}$ :

$$|\alpha_n - \alpha_m| < \epsilon$$

$\alpha_n = \langle f_n, g_n \rangle_{\mathcal{H}_0}$  is convergent by Cauchyness in  $\mathbb{R}$ :

$$\begin{aligned} |\alpha_n - \alpha_m| &= |\langle f_n, g_n \rangle_{\mathcal{H}_0} - \langle f_m, g_m \rangle_{\mathcal{H}_0}| \\ &= |\langle f_n, g_n \rangle_{\mathcal{H}_0} - \langle f_m, g_n \rangle_{\mathcal{H}_0} + \langle f_m, g_n \rangle_{\mathcal{H}_0} - \langle f_m, g_m \rangle_{\mathcal{H}_0}| \\ &= |\langle f_n - f_m, g_n \rangle_{\mathcal{H}_0} + \langle f_m, g_n - g_m \rangle_{\mathcal{H}_0}| \\ &\leq |\langle f_n - f_m, g_n \rangle_{\mathcal{H}_0}| + |\langle f_m, g_n - g_m \rangle_{\mathcal{H}_0}| \\ &\leq \underbrace{\|g_n\|_{\mathcal{H}_0}}_{< A} \underbrace{\|f_n - f_m\|_{\mathcal{H}_0}}_{< \frac{\epsilon}{2A}} + \underbrace{\|f_m\|_{\mathcal{H}_0}}_{< B} \underbrace{\|g_n - g_m\|_{\mathcal{H}_0}}_{< \frac{\epsilon}{2B}} < \epsilon. \end{aligned}$$

$f_n, g_n$ : Cauchy  $\Rightarrow$  bounded, i.e.  $\|f_n\|_{\mathcal{H}_0} < A, \|g_n\|_{\mathcal{H}_0} < B$ .

The limit is independent of the Cauchy seq. chosen: let

- $f_n, f'_n \xrightarrow{\forall x} f; g_n, g'_n \xrightarrow{\forall x} g$ :  $\mathcal{H}_0$ -Cauchy seq.-s,
- $\alpha_n = \langle f_n, g_n \rangle_{\mathcal{H}_0}, \alpha'_n = \langle f'_n, g'_n \rangle_{\mathcal{H}_0}$ .



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- $\alpha_n = \langle f_n, g_n \rangle_{\mathcal{H}_0}$ ,  $\alpha'_n = \langle f'_n, g'_n \rangle_{\mathcal{H}_0}$ .
- 'Repeating' the previous argument:

$$|\alpha_n - \alpha'_n| \leq \underbrace{\|g_n\|_{\mathcal{H}_0}}_{\text{bounded}} \underbrace{\|f_n - f'_n\|_{\mathcal{H}_0}}_{\rightarrow 0} + \underbrace{\|f'_n\|_{\mathcal{H}_0}}_{\text{bounded}} \underbrace{\|g_n - g'_n\|_{\mathcal{H}_0}}_{\rightarrow 0}.$$

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- ' $\rightarrow 0$ ':  $f_n, f'_n \xrightarrow{\forall x} f \Rightarrow f_n - f'_n \xrightarrow{\forall x} 0 \Rightarrow f_n - f'_n \xrightarrow{\mathcal{H}_0} 0$  ( $g_n - g'_n$  similarly).

The 'tricky' bit:

$$\langle f, f \rangle_{\mathcal{H}} = 0 \Rightarrow f = 0.$$

- Let  $f_n \xrightarrow{\forall x} f$   $\mathcal{H}_0$ -Cauchy, and  $\langle f, f \rangle_{\mathcal{H}} = \lim_n \|f_n\|_{\mathcal{H}_0}^2 = 0$ . Then

$$|f(x)| = \lim_{n \rightarrow \infty} |f_n(x)| = \lim_{n \rightarrow \infty} |\delta_x(f_n)| \stackrel{(*)}{\leq} \lim_{n \rightarrow \infty} \underbrace{\|\delta_x\|}_{< \infty} \underbrace{\|f_n\|_{\mathcal{H}_0}}_{\rightarrow 0} = 0,$$

(\*):  $\delta_x$  is continuous on  $\mathcal{H}_0$ .

Until now:  $\langle \cdot, \cdot \rangle_{\mathcal{H}}$  is well-defined & inner product.

Remains:

- 1  $\delta_x$ -s are continuous on  $\mathcal{H}$  ( $\forall x$ ).
- 2  $\mathcal{H}$  is complete.
- 3 The reproducing kernel on  $\mathcal{H}$  is  $k$ .

$\mathcal{H}_0$  is dense in  $\mathcal{H}$ .

- Sufficient to show:  $f_n \xrightarrow{\forall x} f$   $\mathcal{H}_0$ -Cauchy  $\Rightarrow f_n \xrightarrow{\mathcal{H}} f$ .

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- Sufficient to show:  $f_n \xrightarrow{\forall x} f$   $\mathcal{H}_0$ -Cauchy  $\Rightarrow f_n \xrightarrow{\mathcal{H}} f$ .
- Proof: Fix  $\epsilon > 0$ ,
  - $f_n$ :  $\mathcal{H}_0$ -Cauchy  $\Rightarrow \exists N \leq \forall m, n: \|f_m - f_n\|_{\mathcal{H}_0} < \epsilon$ .
  - Fix  $n^* \geq N$ , then  $f_m - f_{n^*} \xrightarrow{\forall x} f - f_{n^*}$ .
  - By the definition of  $\|\cdot\|_{\mathcal{H}}$ :

$$\|f - f_{n^*}\|_{\mathcal{H}}^2 = \lim_{m \rightarrow \infty} \|f_m - f_{n^*}\|_{\mathcal{H}_0}^2 \leq \epsilon^2,$$

i.e.,  $f_n \xrightarrow{\mathcal{H}} f$ .

## $\delta_x$ -s are continuous on $\mathcal{H}$

Sufficient to show:  $\delta_x$  linear is continuous at  $f \equiv 0$ . Fix  $x \in \mathcal{X}$ .

- We have seen:  $\delta_x$  is continuous on  $\mathcal{H}_0$ , i.e.  $\exists \eta$

$$\|g - 0\|_{\mathcal{H}_0} = \|g\|_{\mathcal{H}_0} < \eta \Rightarrow |\delta_x(g) - \delta_x(0)| = |\delta_x(g) - 0| = |g(x)| < \epsilon/2.$$

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- Take  $f \in \mathcal{H}$ :  $\|f\|_{\mathcal{H}} < \eta/2$ . Since  $\mathcal{H}_0 \subset \mathcal{H}$  dense,  $\exists f_N$   $\mathcal{H}_0$ -Cauchy,  $\exists N$

$$|f(x) - f_N(x)| < \epsilon/2 \quad [\Leftarrow f_n \xrightarrow{\forall x} f],$$

$$\|f - f_N\|_{\mathcal{H}} < \eta/2 \quad [\Leftarrow f_n \xrightarrow{\mathcal{H}} f] \Rightarrow$$

$$\|f_N\|_{\mathcal{H}_0} = \|f_N\|_{\mathcal{H}} \leq \underbrace{\|f\|_{\mathcal{H}}}_{< \frac{\eta}{2}} + \underbrace{\|f - f_N\|_{\mathcal{H}}}_{< \frac{\eta}{2}} < \eta.$$



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- With  $g = f_N$  we get  $|f_N(x)| < \frac{\epsilon}{2} \Rightarrow$   
 $|f(x)| \leq \underbrace{|f(x) - f_N(x)|}_{< \frac{\epsilon}{2}} + \underbrace{|f_N(x)|}_{< \frac{\epsilon}{2}} < \epsilon.$

High-level idea: let  $\{f_n\} \subset \mathcal{H}$  be any Cauchy seq.,

- $\exists f(x) := \lim_n f_n(x)$  since
  - $\delta_x$  cont. on  $\mathcal{H} \Rightarrow \{f_n(x)\} \subset \mathbb{R}$  Cauchy seq.  $\Rightarrow$  convergent.

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- Question: is the point-wise limit  $f \in \mathcal{H}$ ?

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  - $\delta_x$  cont. on  $\mathcal{H} \Rightarrow \{f_n(x)\} \subset \mathbb{R}$  Cauchy seq.  $\Rightarrow$  convergent.
- Question: is the point-wise limit  $f \in \mathcal{H}$ ?
- Idea:
  - 1  $\mathcal{H}_0$  dense in  $\mathcal{H} \Rightarrow \exists g_n \in \mathcal{H}_0$  s.t.  $\|g_n - f_n\|_{\mathcal{H}} < \frac{1}{n}$ .
  - 2 We show
    - $g_n \xrightarrow{\forall x} f$ ;  $\{g_n\} \subset \mathcal{H}_0$ : Cauchy seq.  $\Rightarrow f \in \mathcal{H}$ .
    - $f_n \xrightarrow{\mathcal{H}} f$ .

- $g_n \xrightarrow{\forall x} f$ :

$$\begin{aligned} |g_n(x) - f(x)| &\leq |g_n(x) - f_n(x)| + |f_n(x) - f(x)| \\ &= \underbrace{|\delta_x(g_n - f_n)|}_{\rightarrow 0; \delta_x \text{ cont. on } \mathcal{H}} + \underbrace{|f_n(x) - f(x)|}_{\rightarrow 0; f \text{ def.}}. \end{aligned}$$

- $\{g_n\} \subset \mathcal{H}_0$  is Cauchy sequence:

$$\begin{aligned}
 \|g_m - g_n\|_{\mathcal{H}_0} &= \|g_m - g_n\|_{\mathcal{H}} \\
 &\leq \|g_m - f_m\|_{\mathcal{H}} + \|f_m - f_n\|_{\mathcal{H}} + \|f_n - g_n\|_{\mathcal{H}} \\
 &\leq \underbrace{\frac{1}{m} + \frac{1}{n}}_{g_m, g_n \text{ def.}} + \underbrace{\|f_m - f_n\|_{\mathcal{H}}}_{\rightarrow 0; f_n: \mathcal{H}\text{-Cauchy}}.
 \end{aligned}$$

- Finally,  $f_n \xrightarrow{\mathcal{H}} f$ :

$$\|f - f_n\|_{\mathcal{H}} \leq \|f - g_n\|_{\mathcal{H}} + \|g_n - f_n\|_{\mathcal{H}} \leq \overbrace{\|f - g_n\|_{\mathcal{H}}}^{\rightarrow 0: \text{ shown at } \mathcal{H}_0 \text{ dense in } \mathcal{H}} + \overbrace{\frac{1}{n}}^{g_n \text{ def.}}$$

# Final property: the reproducing kernel on $\mathcal{H}$ is $k$

- Let  $f \in \mathcal{H}$ , and  $f_n \xrightarrow{\forall x} f$   $\mathcal{H}_0$ -Cauchy sequence.
- Then,

$$\langle f, k(\cdot, x) \rangle_{\mathcal{H}} \stackrel{(a)}{=} \lim_{n \rightarrow \infty} \langle f_n, k(\cdot, x) \rangle_{\mathcal{H}_0} \stackrel{(b)}{=} \lim_{n \rightarrow \infty} f_n(x) \stackrel{(c)}{=} f(x),$$

where

- (a): definition of  $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ ,
- (b):  $k$  reproducing kernel on  $\mathcal{H}_0$ ,
- (c):  $f_n \xrightarrow{\forall x} f$ .



We have shown that

- RKHS ( $\delta_x$  continuous)  $\Leftrightarrow$  reproducing kernel  $\Leftrightarrow$  kernel (feature view)  $\Leftrightarrow$  positive definite.

$\infty$

- *Moore-Aronszajn theorem:*
  - RKHS construction for a  $k$  pos. def. function.
  - Idea:
    - 1 pre-RKHS:  $\mathcal{H}_0 = \text{span}[\{k(\cdot, x)\}_{x \in \mathcal{X}}]$ ,
    - 2  $\mathcal{H} :=$  pointwise limit of  $\mathcal{H}_0$ -Cauchy sequences.

# Appendix

# Vector space axioms

$(V, +, \lambda \cdot)$  is vector space if  $[\forall \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v} \in V, a, b \in \mathbb{R}]$ :

$$(\mathbf{v}_1 + \mathbf{v}_2) + \mathbf{v}_3 = \mathbf{v}_1 + (\mathbf{v}_2 + \mathbf{v}_3), \text{ (associativity)}$$

$$\mathbf{v}_1 + \mathbf{v}_2 = \mathbf{v}_2 + \mathbf{v}_1, \text{ (commutativity)}$$

$$\exists \mathbf{0} : \mathbf{v} + \mathbf{0} = \mathbf{v},$$

$$\exists -\mathbf{v} : \mathbf{v} + (-\mathbf{v}) = \mathbf{0},$$

$$a(b\mathbf{v}) = (ab)\mathbf{v},$$

$$1\mathbf{v} = \mathbf{v},$$

$$a(\mathbf{v}_1 + \mathbf{v}_2) = a\mathbf{v}_1 + a\mathbf{v}_2,$$

$$(a + b)\mathbf{v} = a\mathbf{v} + b\mathbf{v}.$$

# $\mathcal{H}$ is a vector space

$\mathcal{H} \subset \mathbb{R}^X \Rightarrow$  Needed:

①  $f \in \mathcal{H} \Rightarrow \lambda f \in \mathcal{H}$ :  $\exists \{f_n\} \subset \mathcal{H}_0$ -Cauchy,  $f_n \xrightarrow{\forall x} f$ .

$\{\lambda f_n\} \subset \mathcal{H}_0$  ( $\Leftarrow \mathcal{H}_0$ : vector space), Cauchy,  
 $(\lambda f_n)(x) \xrightarrow{\forall x} (\lambda f)(x)$ .

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$$(\lambda f_n)(x) \xrightarrow{\forall x} (\lambda f)(x).$$

②  $f, g \in \mathcal{H} \Rightarrow f + g \in \mathcal{H}: \exists \{f_n\}, \{g_n\} \subset \mathcal{H}_0$ -Cauchy,  $f_n \xrightarrow{\forall x} f, g_n \xrightarrow{\forall x} g$

$$\{f_n + g_n\} \subset \mathcal{H}_0 (\Leftarrow \mathcal{H}_0: \text{vector space}), \text{Cauchy,}$$

$$(f_n + g_n)(x) \xrightarrow{\forall x} (f + g)(x).$$

## $\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$ : inner product

Needed: for  $\forall f = \sum_i \alpha_i k(\cdot, x_i), g = \sum_j \beta_j k(\cdot, y_j) \in \mathcal{H}_0$

①  $\langle f, g \rangle_{\mathcal{H}_0} = \langle g, f \rangle_{\mathcal{H}_0}$ :

$$\langle f, g \rangle_{\mathcal{H}_0} = \sum_i \sum_j \alpha_i \beta_j k(x_i, y_j) = \sum_j \sum_i \beta_j \alpha_i k(y_j, x_i) = \langle g, f \rangle_{\mathcal{H}_0}.$$

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③  $\langle f_1 + f_2, g \rangle_{\mathcal{H}_0} = \langle f_1, g \rangle_{\mathcal{H}_0} + \langle f_2, g \rangle_{\mathcal{H}_0}$  [ $f_1 \leftrightarrow \alpha'_i, x'_i, f_2 \leftrightarrow \alpha''_i, x''_i$ ]:

$$\text{l.h.s} = \sum_{i,j} \alpha_i \beta_j k(x_i, y_j) = \sum_{i,j} \alpha'_i \beta_j k(x'_i, y_j) + \sum_{i,j} \alpha''_i \beta_j k(x''_i, y_j) = \text{r.h.s.},$$

where  $f_1 + f_2 \leftrightarrow \alpha'_i, \alpha''_i, x'_i, x''_i$ .



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where  $f_1 + f_2 \leftrightarrow \alpha'_i, \alpha''_i, x'_i, x''_i$ .

④  $f = 0 \Rightarrow \langle f, f \rangle_{\mathcal{H}_0} = 0$ :

$$f = 0 \times k(\cdot, x) \Rightarrow \langle f, f \rangle_{\mathcal{H}_0} = 0 \times 0 \times k(x, x) = 0.$$

## $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ : semi-inner product

Needed: for  $\forall f, f_1, f_2, g \in \mathcal{H}$

①  $\langle f, g \rangle_{\mathcal{H}} = \langle g, f \rangle_{\mathcal{H}}$ :

$$\langle f, g \rangle_{\mathcal{H}} = \lim_n \langle f_n, g_n \rangle_{\mathcal{H}_0} \stackrel{\mathcal{H}_0: \checkmark}{=} \lim_n \langle g_n, f_n \rangle_{\mathcal{H}_0} = \langle g, f \rangle_{\mathcal{H}}.$$

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$$\begin{aligned} \langle f_1 + f_2, g \rangle_{\mathcal{H}} &= \lim_n \langle f_{1,n} + f_{2,n}, g \rangle_{\mathcal{H}_0} \stackrel{\mathcal{H}_0: \checkmark}{=} \lim_n [\langle f_{1,n}, g \rangle_{\mathcal{H}_0} + \langle f_{2,n}, g \rangle_{\mathcal{H}_0}] \\ &= \lim_n \langle f_{1,n}, g \rangle_{\mathcal{H}_0} + \lim_n \langle f_{2,n}, g \rangle_{\mathcal{H}_0} = \langle f_1, g \rangle_{\mathcal{H}} + \langle f_2, g \rangle_{\mathcal{H}}. \end{aligned}$$

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④  $f = 0 \Rightarrow \langle f, f \rangle_{\mathcal{H}} = 0$ : Let  $f_n \equiv 0$

$$\langle f, f \rangle_{\mathcal{H}} = \lim_n \langle 0, 0 \rangle_{\mathcal{H}_0} \stackrel{\mathcal{H}_0: \checkmark}{=} \lim_n 0 = 0.$$