A SUPPLEMENTARY MATERIAL

This supplementary material contains (i) detailed proofs of the consistency of MERR (Section A.1), (ii) numerical illustrations (Section A.2).

A.1 Proofs

A.1.1 Proof of k: continuous, bounded $\Rightarrow$ μ: H-measurable; μ: H-measurable, $X = \mu(\mathcal{M}_1^+(\mathcal{X})) \in \mathcal{B}(H) \Rightarrow \mu$: X-measurable $\Rightarrow \exists\rho$

Below we give sufficient conditions for the existence of probability measure ρ. We divide the proof into 3 steps:

- **k: continuous, bounded $\Rightarrow$ μ: H-measurable**: The mapping $\mu : (\mathcal{M}_1^+(\mathcal{X}), \mathcal{B}(\tau_w)) \to (H, \mathcal{B}(H))$ is measurable, iff the $L_h : (\mathcal{M}_1^+(\mathcal{X}), \mathcal{B}(\tau_w)) \to (\mathbb{R}, \mathcal{B}(\mathbb{R}))$ map defined as $L_h(x) = \langle h, \mu_x \rangle_H \left(= \int_{\mathcal{X}} h(u)\mathrm{d}x(u)\right)$ is measurable for $\forall h \in H$ [38, Theorem IV. 22, page 116]. If k is assumed to be continuous and bounded, these properties also hold for $\forall h \in H$ [6, Lemma 4.23, page 124; Lemma 4.28, page 128], i.e. $H = H(k) \subseteq C_b(\mathcal{X})$. By the definition of the weak topology the L_h functions are continuous (for $\forall h \in H$), which implies the required Borel measurability [6, page 480] of L_h-s (for $\forall h \in H$).
- **$\mu : H$-measurable, $X = \mu(\mathcal{M}_1^+(\mathcal{X}) \in \mathcal{B}(H) \Rightarrow \mu : X$-measurable**: Let τ denote the open sets on $H = H(k)$. Let $\tau|_X = \{A \cap X : A \in \tau\}$ be the subspace topology on X, and let $\mathcal{B}(H)|_X = \{A \cap X : A \in \mathcal{B}(H)\}$ be the subspace σ-algebra on X. Since $\mathcal{B}(\tau|_X) = \mathcal{B}(H)|_X \subseteq \mathcal{B}(H)$ (the containing relation follows from the $X \in \mathcal{B}(H)$ condition), and $\mathcal{B}(H)|_X = \{A \in \mathcal{B}(H) : A \subseteq X\}$, the measurability of $\mu : (\mathcal{M}_1^+(\mathcal{X}), \mathcal{B}(\tau_w)) \to (H, \mathcal{B}(H))$ implies the measurability of $\mu : (\mathcal{M}_1^+(\mathcal{X}), \mathcal{B}(\tau_w)) \to (X, \mathcal{B}(H)|_X)$.
- **$\mu : X$-measurable $\Rightarrow \exists\rho$**: Let us consider the

$$g : (\mathcal{M}_1^+(\mathcal{X}) \times \mathbb{R}, \mathcal{B}(\tau_w) \otimes \mathcal{B}(\mathbb{R})) \to (X \times \mathbb{R},\ \mathcal{B}(H)|_X \otimes \mathcal{B}(\mathbb{R})) \tag{14}$$

$g(x, y) = [g_1(x, y); g_2(x, y)] = [\mu_x; y]$ mapping. If g is a *measurable* function, then it defines ρ, a probability measure on $(X \times \mathbb{R},\ \mathcal{B}(H)|_X \otimes \mathcal{B}(\mathbb{R}))$ by looking at g as a random variable taking values in $X \times \mathbb{R}$:

$$\rho(C) := \mathcal{M}\left(g^{-1}(C)\right), \quad (C \in \mathcal{B}(H)|_X \otimes \mathcal{B}(\mathbb{R})). \tag{15}$$

Function g in Eq. (14) is measurable iff its coordinate functions, g_1 and g_2 are both measurable functions [39, Proposition 3.2, page 201]. Thus, we need for $\forall A \in \mathcal{B}(H)|_X$, $\forall B \in \mathcal{B}(\mathbb{R})$

$$\mathcal{B}(\tau_w) \otimes \mathcal{B}(\mathbb{R}) \ni g_1^{-1}(A) = \{(x, y) : g_1(x, y) = \mu_x \in A\} = \mu^{-1}(A) \times \mathbb{R}, \tag{16}$$

$$\mathcal{B}(\tau_w) \otimes \mathcal{B}(\mathbb{R}) \ni g_2^{-1}(B) = \{(x, y) : g_2(x, y) = y \in B\} = \mathcal{M}_1^+(\mathcal{X}) \times B. \tag{17}$$

According to Eqs. (16)-(17), the measurability of g follows from the X-measurability of $\mu : (\mathcal{M}_1^+(\mathcal{X}), \mathcal{B}(\tau_w)) \to (X, \mathcal{B}(H)|_X)$, which is guaranteed by our conditions.

A.1.2 Proof of Ψ: Hölder continuous $\Rightarrow$ K: measurable

[5]'s original assumption that $(\mu_a, \mu_b) \in X \times X \mapsto K(\mu_a, \mu_b) \in \mathbb{R}$ is measureable follows from the required Hölder continuity [see Eq. (5)] since (i) the continuity of Ψ is equivalent to that of K, (ii) a continuous map between topological spaces is Borel measurable [6, Lemma 4.29 on page 128; page 480].

A.1.3 Proof of K: linear $\Rightarrow$ Ψ: Hölder continuous with $L = 1$, $h = 1$

In case of a linear K kernel $K(\mu_a, \mu_b) = \langle \mu_a, \mu_b \rangle_H \quad (\mu_a, \mu_b \in X)$, by the bilinearity of $\langle \cdot, \cdot \rangle_H$ and $\|\langle \cdot, a \rangle_H\|_{\mathcal{H}}^2 = \|a\|_H^2$, we get that $\|K(\cdot, \mu_a) - K(\cdot, \mu_b)\|_{\mathcal{H}} = \|\langle \cdot, \mu_a \rangle_H - \langle \cdot, \mu_b \rangle_H\|_{\mathcal{H}} = \|\langle \cdot, \mu_a - \mu_b \rangle_H\|_{\mathcal{H}} = \|\mu_a - \mu_b\|_H$. In other words, Hölder continuity holds with $L = 1$, $h = 1$; K is Lipschitz continuous ($h = 1$).

A.1.4 Proof of $\mathcal{X}$: compact metric, μ: continuous $\Rightarrow$ $X = \mu\left(\mathcal{M}_1^+(\mathcal{X})\right)$: compact metric

Let us suppose that $\mathcal{X} = (\mathcal{X}, d)$ is a compact metric space. This implies that $\mathcal{M}_1^+(\mathcal{X})$ is also a compact metric space by Theorem 6.4 in [40] (page 55). The continuous (μ) image of a compact set is compact (see page 478 in [6]), thus $X = \mu\left(\mathcal{M}_1^+(\mathcal{X})\right) \subseteq H$ is compact metric.

A.1.5 Proof of the Kernel Examples on $X = \mu(\mathcal{M}_1^+(\mathcal{X}))$

Below we prove for the $K : X \times X \to \mathbb{R}$ functions in Table 1 that they are kernels on mean embedded distributions.

We need some definitions and lemmas. $\mathbb{Z}, \mathbb{Z}^+, \mathbb{R}^+, \mathbb{R}^{\geq 0}$ denotes the set of integers, positive integers, positive real numbers and non-negative real numbers, respectively.

Definition 1. *Let X be a non-empty set. A $K : X \times X \to \mathbb{R}$ function is called*

- positive definite *(pd; also referred to as kernel) on X, if it is*
  1. *symmetric [$K(a,b) = K(b,a)$, $\forall a, b \in X$], and*
  2. *$\sum_{i,j=1}^n c_i c_j K(a_i, a_j) \geq 0$ for all $n \in \mathbb{Z}^+$, $\{a_1, \ldots, a_n\} \subseteq X^n$, $\mathbf{c} = [c_1; \ldots; c_n] \in \mathbb{R}^n$.*
- negative definite *(nd; sometimes $-K$ is called conditionally positive definite) on X, if it is*
  1. *symmetric, and*
  2. *$\sum_{i,j=1}^n c_i c_j K(a_i, a_j) \leq 0$ for all $n \in \mathbb{Z}^+$, $\{a_1, \ldots, a_n\} \subseteq X^n$, $\mathbf{c} = [c_1; \ldots; c_n] \in \mathbb{R}^n$, where $\sum_{j=1}^n c_j = 0$.*

We will use the following properties of positive/negative definite functions:

1. K is nd $\Leftrightarrow$ e^{-tK} is pd for all $t > 0$; see Chapter 3 in [33].
2. $K : X \times X \to \mathbb{R}^{\geq 0}$ is nd $\Leftrightarrow$ $\frac{1}{t+K}$ is pd for all $t > 0$; see Chapter 3 in [33].
3. If K is nd and non-negative on the diagonal ($K(x,x) \geq 0$, $\forall x \in X$), then K^α is nd for all $\alpha \in [0,1]$; see Chapter 3 in [33].
4. $K(x,y) = \langle x, y \rangle_X$ is pd, where X is a Hilbert space (since the pd property is equivalent to being a kernel).
5. $K(x,y) = \|x - y\|_X^2$ is nd, where X is a Hilbert space; see Chapter 3 in [33].
6. If K is nd, $K + d$ ($d \in \mathbb{R}$) is also nd. Proof: (i) $K(x,y) + d = K(y,x) + d$ holds by the symmetry of K, (ii) $\sum_{i,j=1}^n c_i c_j \left[K(a_i, a_j) + d\right] = \sum_{i,j=1}^n c_i c_j K(a_i, a_j) + \sum_{i=1}^n c_i \sum_{j=1}^n c_j d = \sum_{i,j=1}^n c_i c_j K(a_i, a_j) + \sum_{i=1}^n c_i d \sum_{j=1}^n c_j = \sum_{i,j=1}^n c_i c_j K(a_i, a_j) + 0 \leq 0$, where we used that $\sum_{j=1}^n c_j = 0$ and K is nd.
7. If K is pd (nd) on X, then it is pd (nd) on $X' \subseteq X$ as well. Proof: less constraints have to be satisfied for $X' \subseteq X$.
8. If K is pd (nd) on X, then sK ($s \in \mathbb{R}^+$) is also pd (nd). Proof: multiplication by a positive constant does not affect the sign of $\sum_{i,j=1}^n c_i c_j K(a_i, a_j)$.
9. If K is nd on X and $K(x,y) > 0$ $\forall x, y \in X$, then $\frac{1}{K}$ is pd; see Chapter 3 in [33].
10. If K is pd on X, and $h(u) = \sum_{n=0}^\infty a_n u^n$ with $a_n \geq 0$, then $h \circ K$ is pd; see Chapter 3 in [33].

Making use of these properties one can prove the kernel property of the K-s in Table 1 (see also Table 3) as follows. All the K-s are functions of $\|\mu_a - \mu_b\|_H$, $\|\mu_a - \mu_b\|_H = \|\mu_b - \mu_a\|_H$, hence K-s are symmetric.

$K(x,y) = \|x - y\|_H^2$ is nd on $H = H(k)$ (Prop. 5), thus $K(x,y) = \|x - y\|_H^2$ is nd on $X = \mu\left(\mathcal{M}_1^+(\mathcal{X})\right) \subseteq H(k)$ (Prop. 7). Consequently, $K(x,y) = \|x - y\|_H^d$ is nd on X, where $d \in [0,2]$ ($K(x,x) = 0 \geq 0$, Prop. 3).

- Hence, $K(x,y) = e^{-t\|x-y\|_H^d}$ is pd, where $t > 0$, $d \in [0,2]$ (Prop. 1). By the $(t,d) = \left(\frac{1}{2\theta^2}, 2\right)$ and $(t,d) = \left(\frac{1}{2\theta^2}, 1\right)$ choices, we get that K_G and K_e are kernels.
- Using Prop. 2 ($\|x - y\|_H^d \geq 0$), one obtains that $K(x,y) = \frac{1}{t + \|x-y\|_H^d}$ is pd on X, where $t > 0$, $d \in [0,2]$. By the $(t,d) = (1, \leq 2)$ choice the kernel property of K_t follows.
- Thus, $K(x,y) = s\|x - y\|_H^d$ is nd on X, where $s > 0$, $d \in [0,2]$ (Prop. 8). Consequently, $K(x,y) = \frac{1}{t + s\|x-y\|_H^d}$ is pd on X, where $s > 0$, $d \in [0,2]$, $t > 0$ (Prop. 2). By the $(d,t,s) = (2, 1, \frac{1}{\theta^2})$, we have that K_C is kernel.
- Hence, $K(x,y) = \|x - y\|_H^d + e$ is nd on X, where $d \in [0,2]$, $e \in \mathbb{R}^+$ (Prop. 6). Thus, $K(x,y) = \left(\|x - y\|_H^d + e\right)^f$ is nd on X, where $d \in [0,2]$, $e \in \mathbb{R}^+$, $f \in (0,1]$ ($\|x - y\|_H^d + e \geq 0$, Prop. 3). Consequently, $K(x,y) = \frac{1}{\left(\|x-y\|_H^d + e\right)^f}$ is pd on X, where $d \in [0,2]$, $e \in \mathbb{R}^+$, $f \in (0,1]$ ($\left(\|x - y\|_H^d + e\right)^f > 0$; Prop. 9); with the $(d,e,f) = \left(2, \theta^2, \frac{1}{2}\right)$ choice, one obtains that K_i is a kernel.

A.1.6 Proof of "Conditions of Proof A.1.4 and Proof A.1.5" $\Rightarrow$ Ψ-s of K-s in Proof A.1.5: Hölder continuous

We tackle the problem more generally:

Table 3: Nonlinear kernels on mean embedded distributions.

Kernel (K)	Parameter(s)
$K(\mu_a,\mu_b)=e^{-t\|\mu_a-\mu_b\|_H^d}$	$t>0$, $d\in[0,2]$
$K(\mu_a,\mu_b)=\frac{1}{t+\|\mu_a-\mu_b\|_H^d}$	$t>0$, $d\in[0,2]$
$K(\mu_a,\mu_b)=\frac{1}{t+s\|\mu_a-\mu_b\|_H^d}$	$s>0$, $d\in[0,2]$, $t>0$
$K(\mu_a,\mu_b)=\frac{1}{(\|\mu_a-\mu_b\|_H^d+e)^f}$	$d\in[0,2]$, $e\in\mathbb{R}^+$

1. we give sufficient conditions for K kernels of the form

$$K(\mu_a,\mu_b)=\bar{K}\left(\|\mu_a-\mu_b\|_H\right), \tag{18}$$

   i.e., for radial kernels to have Hölder continuous canonical feature map ($\Psi(\mu_c)=K(\cdot,\mu_c)$): $\exists L>0$, $h\in(0,1]$ such that $\|K(\cdot,\mu_a)-K(\cdot,\mu_b)\|_{\mathcal{H}}\leq L\|\mu_a-\mu_b\|_H^h$.
2. Then we show that these sufficient conditions are satisfied for the K kernels listed in Table 1.

Let us first note that K is bounded. Indeed, since Ψ is Hölder continuous, specially it is continuous. Hence using Lemma 4.29 in [6] (page 128), the

$$K_0:\mu_a\in X\to K(\mu_a,\mu_a)\in\mathbb{R}$$

mapping is continuous. As we have already seen (Section A.1.4) X is compact. The continuous (K_0) image of a compact set (X), i.e., the $\{K(\mu_a,\mu_a):\mu_a\in X\}\subseteq\mathbb{R}$ set is compact, specially it is bounded above.

1. Sufficient conditions: Now, we present sufficient conditions for the assumed Hölder continuity

$$\|K(\cdot,\mu_a)-K(\cdot,\mu_b)\|_{\mathcal{H}}\leq L\|\mu_a-\mu_b\|_H^h. \tag{19}$$

   Using $\|u\|_{\mathcal{H}}^2=\langle u,u\rangle_{\mathcal{H}}$, the bilinearity of $\langle\cdot,\cdot\rangle_{\mathcal{H}}$, the reproducing property of K and Eq. (18), we get

$$\begin{aligned}\|K(\cdot,\mu_a)-K(\cdot,\mu_b)\|_{\mathcal{H}}^2&=\langle K(\cdot,\mu_a)-K(\cdot,\mu_b),K(\cdot,\mu_a)-K(\cdot,\mu_b)\rangle_{\mathcal{H}}\\&=K(\mu_a,\mu_a)+K(\mu_b,\mu_b)-2K(\mu_a,\mu_b)=2\bar{K}(0)-2\bar{K}(\|\mu_a-\mu_b\|_H)\\&=2\left[\bar{K}(0)-\bar{K}\left(\|\mu_a-\mu_b\|_H\right)\right].\end{aligned}$$

   Hence, the Hölder continuity of K is equivalent to the existence of an $L'\left(=\frac{L^2}{2}\right)>0$ such that

$$\bar{K}(0)-\bar{K}\left(\|\mu_a-\mu_b\|_H\right)\leq L'\|\mu_a-\mu_b\|_H^{2h}.$$

   Since for $\mu_a=\mu_b$ both sides are equal to 0, this requirement is equivalent to

$$u(\mu_a,\mu_b):=\frac{\bar{K}(0)-\bar{K}\left(\|\mu_a-\mu_b\|_H\right)}{\|\mu_a-\mu_b\|_H^{2h}}\leq L',\quad(\mu_a\neq\mu_b)$$

   i.e., that the $u:X\times X\to\mathbb{R}$ function is bounded above. Function u is the composition ($u=u_2\circ u_1$) of the mappings:

$$\begin{aligned}&u_1:X\times X\to\mathbb{R}^{\geq 0},\quad u_1(\mu_a,\mu_b)=\|\mu_a-\mu_b\|_H,\\&u_2:\mathbb{R}^{\geq 0}\to\mathbb{R},\quad u_2(v)=\frac{\bar{K}(0)-\bar{K}(v)}{v^{2h}}.\end{aligned} \tag{20}$$

   Here, u_1 is continuous. Let us *suppose* for u_2 that
   (a) (i) $\exists h\in(0,1]$ such that $\lim_{v\to 0+}u_2(v)$ exists, and
   (b) u_2 is continuous.

In this case, since the composition of continuous functions is continuous (see page 85 in [41]), u is continuous. As we have seen (Section A.1.4), X is compact. The product of compact sets $(X \times X)$ is compact by the Tychonoff theorem (see page 143 in [41]). Finally, since the continuous (u) image of a compact set $(X \times X)$, i.e. $\{u(\mu_a, \mu_b) : (\mu_a, \mu_b) \in X \times X\} \subseteq \mathbb{R}$ is compact (Theorem 8 in [41], page 141), we get that u is bounded, specially bounded above.

To sum up, we have proved that if

(a) K is radial [see Eq. (18)],

(b) u_2 [Eq. (20)] is (i) continuous and (ii) $\exists h \in (0, 1]$ such that $\lim_{v\to 0+} u_2(v)$ exists,

then the Hölder property [Eq. (19)] holds for K with exponent h. In other words, the Hölder property of a kernel K on mean embedded distributions can be simply guaranteed by the appropriate behavior of $\bar{K}$ at zero.

2. Verification of the sufficient conditions: In the sequel we show that these conditions hold for the u_2 functions of the K kernels in Table 1. In the examples

$$\bar{K}_G(v) = e^{-\frac{v^2}{2\theta^2}}, \qquad \bar{K}_e(v) = e^{-\frac{v}{2\theta^2}}, \qquad \bar{K}_C(v) = \frac{1}{1+\frac{v^2}{\theta^2}}, \qquad \bar{K}_t(v) = \frac{1}{1+v^\theta}, \qquad \bar{K}_i(v) = \frac{1}{\sqrt{v^2+\theta^2}}.$$

The corresponding u_2 functions are

$$u_{2G}(v) = \frac{1-e^{-\frac{v^2}{2\theta^2}}}{v^{2h}}, \quad u_{2e}(v) = \frac{1-e^{-\frac{v}{2\theta^2}}}{v^{2h}}, \quad u_{2C}(v) = \frac{1-\frac{1}{1+\frac{v^2}{\theta^2}}}{v^{2h}}, \quad u_{2t}(v) = \frac{1-\frac{1}{1+v^\theta}}{v^{2h}}, \quad u_{2i}(v) = \frac{\frac{1}{\theta}-\frac{1}{\sqrt{v^2+\theta^2}}}{v^{2h}}.$$

The limit requirements at zero complementing the continuity of u_2-s are satisfied:

- u_{2G}: In this case

$$\lim_{v\to 0+} u_{2G}(v) = \lim_{v\to 0+} \frac{1-e^{-\frac{v^2}{2\theta^2}}}{v^2} = \lim_{v\to 0+} \frac{1-e^{-\frac{v}{2\theta^2}}}{v} = \lim_{v\to 0+} \frac{\frac{1}{2\theta^2}e^{-\frac{v}{2\theta^2}}}{1} = \frac{1}{2\theta^2},$$

  where we applied a v^2 substitution and the L'Hopital rule; $h = 1$.

- u_{2e}:

$$\lim_{v\to 0+} u_{2e}(v) = \lim_{v\to 0+} \frac{1-e^{-\frac{v}{2\theta^2}}}{v^{2h}} = \lim_{v\to 0+} \frac{\frac{1}{2\theta^2}e^{-\frac{v}{2\theta^2}}}{2hv^{2h-1}} = \frac{1}{2\theta^2},$$

  where we applied the L'Hopital rule and chose $h = \frac{1}{2}$, the largest h from the $2h - 1 \leq 0$ convergence domain.

- u_{2C}:

$$u_{2C}(v) = \frac{1-\frac{1}{1+\frac{v^2}{\theta^2}}}{v^{2h}} = \frac{1-\frac{\theta^2}{\theta^2+v^2}}{v^{2h}} = \frac{\frac{v^2}{\theta^2+v^2}}{v^{2h}} = \frac{v^{2-2h}}{\theta^2+v^2 \xrightarrow{v\to 0+} \theta^2},$$

  we chose $h = 1$, the largest value from the convergence domain $(2 - 2h \geq 0 \Rightarrow 1 \geq h)$.

- u_{2t}:

$$u_{2t}(v) = \frac{1-\frac{1}{1+v^\theta}}{v^{2h}} = \frac{v^{\theta-2h}}{1+v^\theta \xrightarrow{v\to 0} 1},$$

  thus we can have $h = \frac{\theta}{2}$, the largest element of the convergence domain $(\theta - 2h \geq 0 \Leftrightarrow \frac{\theta}{2} \geq h)$. Here we require $\theta \leq 2$ in order to guarantee that $h = \frac{\theta}{2} \leq 1$.

- u_{2i}: Let g denote the nominator of u_{2i}

$$\begin{aligned} g(v) &= \frac{1}{\theta} - \frac{1}{\sqrt{v^2+\theta^2}} = \frac{1}{\theta} - \left[g(0) + g'(0)v + \frac{g''(0)}{2}v^2 + \dots\right] \\ &= \frac{1}{\theta} - \left[\frac{1}{\theta} + \left(-\frac{1}{2}\frac{1}{(v^2+\theta)^{\frac{3}{2}}}2v\right)\Big|_{v=0} v + \frac{g''(0)}{2}v^2 + \dots\right] = -v^2\left[\frac{g''(0)}{2!} + \frac{g^{(3)}(0)}{3!}v + \dots\right]. \end{aligned}$$

  Hence,

$$\lim_{v\to 0+} u_{2i}(v) = \lim_{v\to 0+} \frac{\frac{1}{\theta}-\frac{1}{\sqrt{v^2+\theta^2}}}{v^2} = \lim_{v\to 0+} \frac{-v^2\left[\frac{g''(0)}{2!} + \frac{g^{(3)}(0)}{3!}v + \dots\right]}{v^2} = -\frac{g''(0)}{2},$$

  i.e., h can be chosen to be 1 ($h = 1$).

A.1.7 Proof of $\|\sum_{i=1}^n f_i\|^2 \le n\sum_{i=1}^n \|f_i\|^2$

In a normed space $(N, \|\cdot\|)$

$$\left\|\sum_{i=1}^n f_i\right\|^2 \le n\sum_{i=1}^n \|f_i\|^2, \tag{21}$$

where $f_i \in N$ $(i = 1, \dots, n)$.

Indeed the statement holds since $\|\sum_{i=1}^n f_i\|^2 \le (\sum_{i=1}^n \|f_i\|)^2 \le n\sum_{i=1}^n \|f_i\|^2$, where we applied the triangle inequality, and a consequence that the arithmetic mean is smaller or equal than the squared mean (special case of the generalized mean inequality) with $a_i = \|f_i\| \ge 0$. Particularly, $\frac{\sum_{i=1}^n a_i}{n} \le \sqrt{\frac{\sum_{i=1}^n (a_i)^2}{n}} \Rightarrow (\sum_{i=1}^n a_i)^2 \le n\sum_{i=1}^n (a_i)^2$.

A.1.8 Proof of the Decomposition of the Excess Risk

It is known [5] that $\mathcal{E}[f] - \mathcal{E}[f_{\mathcal{H}}] = \|\sqrt{T}(f - f_{\mathcal{H}})\|_{\mathcal{H}}^2 \quad (\forall f \in \mathcal{H})$. Applying this identity with $f = f_{\hat{\mathbf{z}}}^{\lambda} \in \mathcal{H}$ and a telescopic trick, we get

$$\mathcal{E}\left[f_{\hat{\mathbf{z}}}^{\lambda}\right] - \mathcal{E}\left[f_{\mathcal{H}}\right] = \left\|\sqrt{T}\left(f_{\hat{\mathbf{z}}}^{\lambda} - f_{\mathcal{H}}\right)\right\|_{\mathcal{H}}^2 = \left\|\sqrt{T}\left[\left(f_{\hat{\mathbf{z}}}^{\lambda} - f_{\mathbf{z}}^{\lambda}\right) + \left(f_{\mathbf{z}}^{\lambda} - f^{\lambda}\right) + \left(f^{\lambda} - f_{\mathcal{H}}\right)\right]\right\|_{\mathcal{H}}^2. \tag{22}$$

By Eqs. (9), (10), and the operator identity $A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}$ one obtains for the first term in Eq. (22)

$$\begin{aligned} f_{\hat{\mathbf{z}}}^{\lambda} - f_{\mathbf{z}}^{\lambda} &= (T_{\hat{\mathbf{x}}} + \lambda)^{-1} g_{\hat{\mathbf{z}}} - (T_{\mathbf{x}} + \lambda)^{-1} g_{\mathbf{z}} = (T_{\hat{\mathbf{x}}} + \lambda)^{-1}(g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}) + (T_{\hat{\mathbf{x}}} + \lambda)^{-1} g_{\mathbf{z}} - (T_{\mathbf{x}} + \lambda)^{-1} g_{\mathbf{z}} \\ &= (T_{\hat{\mathbf{x}}} + \lambda)^{-1}(g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}) + \left[(T_{\hat{\mathbf{x}}} + \lambda)^{-1} - (T_{\mathbf{x}} + \lambda)^{-1}\right] g_{\mathbf{z}} \\ &= (T_{\hat{\mathbf{x}}} + \lambda)^{-1}(g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}) + \left[(T_{\hat{\mathbf{x}}} + \lambda)^{-1}(T_{\mathbf{x}} - T_{\hat{\mathbf{x}}})(T_{\mathbf{x}} + \lambda)^{-1}\right] g_{\mathbf{z}} \\ &= (T_{\hat{\mathbf{x}}} + \lambda)^{-1}\left[(g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}) + (T_{\mathbf{x}} - T_{\hat{\mathbf{x}}})(T_{\mathbf{x}} + \lambda)^{-1} g_{\mathbf{z}}\right] = (T_{\hat{\mathbf{x}}} + \lambda)^{-1}\left[(g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}) + (T_{\mathbf{x}} - T_{\hat{\mathbf{x}}}) f_{\mathbf{z}}^{\lambda}\right]. \end{aligned}$$

Thus, we can rewrite the first term in (22) as

$$\sqrt{T}\left(f_{\hat{\mathbf{z}}}^{\lambda} - f_{\mathbf{z}}^{\lambda}\right) =: f_{-1} + f_0, \qquad f_{-1} = \sqrt{T}(T_{\hat{\mathbf{x}}} + \lambda)^{-1}(g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}), \qquad f_0 = \sqrt{T}(T_{\hat{\mathbf{x}}} + \lambda)^{-1}(T_{\mathbf{x}} - T_{\hat{\mathbf{x}}}) f_{\mathbf{z}}^{\lambda}.$$

The second term in (22) can be decomposed [5] as

$$\begin{aligned} \sqrt{T}\left[\left(f_{\mathbf{z}}^{\lambda} - f^{\lambda}\right) + \left(f^{\lambda} - f_{\mathcal{H}}\right)\right] &= \sqrt{T}\left[(T_{\mathbf{x}} + \lambda)^{-1}(g_{\mathbf{z}} - T_{\mathbf{x}} f_{\mathcal{H}}) + (T_{\mathbf{x}} + \lambda)^{-1}(T - T_{\mathbf{x}})(f^{\lambda} - f_{\mathcal{H}}) + (f^{\lambda} - f_{\mathcal{H}})\right] \\ &=: f_1 + f_2 + f_3, \end{aligned}$$

where

$$f_1 = \sqrt{T}(T_{\mathbf{x}} + \lambda)^{-1}(g_{\mathbf{z}} - T_{\mathbf{x}} f_{\mathcal{H}}), \qquad f_2 = \sqrt{T}(T_{\mathbf{x}} + \lambda)^{-1}(T - T_{\mathbf{x}})(f^{\lambda} - f_{\mathcal{H}}), \qquad f_3 = \sqrt{T}(f^{\lambda} - f_{\mathcal{H}}).$$

Using these f_i notations, (22) can be upper bounded as

$$\mathcal{E}\left[f_{\hat{\mathbf{z}}}^{\lambda}\right] - \mathcal{E}\left[f_{\mathcal{H}}\right] = \left\|\sum_{i=-1}^{3} f_i\right\|_{\mathcal{H}}^2 \le 5\sum_{i=-1}^{3} \|f_i\|_{\mathcal{H}}^2, \tag{23}$$

exploiting Section A.1.7 ($\|\cdot\|^2 = \|\cdot\|_{\mathcal{H}}^2$, $n = 5$). Consequently, introducing the

$$\begin{aligned} S_{-1} &= S_{-1}(\lambda, \mathbf{z}, \hat{\mathbf{z}}) = \|f_{-1}\|_{\mathcal{H}}^2, & S_0 &= S_0(\lambda, \mathbf{z}, \hat{\mathbf{z}}) = \|f_0\|_{\mathcal{H}}^2, \\ S_1 &= S_1(\lambda, \mathbf{z}) = \|f_1\|_{\mathcal{H}}^2, & S_2 &= S_2(\lambda, \mathbf{z}) = \|f_2\|_{\mathcal{H}}^2, & \mathcal{A}(\lambda) &= \|f_3\|_{\mathcal{H}}^2, \end{aligned}$$

notations (for $\mathcal{A}(\lambda)$ see also Theorem 4), (23) can be rewritten as

$$\mathcal{E}\left[f_{\hat{\mathbf{z}}}^{\lambda}\right] - \mathcal{E}\left[f_{\mathcal{H}}\right] \le 5\left[S_{-1} + S_0 + \mathcal{A}(\lambda) + S_1 + S_2\right]. \tag{24}$$

A.1.9 Proof of the Upper Bounding Terms of S_{-1} and S_0

Using the

$$\|Mu\|_{\mathcal{H}} \leq \|M\|_{\mathcal{L}(\mathcal{H})}\|u\|_{\mathcal{H}} \quad (M \in \mathcal{L}(\mathcal{H}), u \in \mathcal{H}), \tag{25}$$

relation, we get

$$S_{-1} \leq \left\|\sqrt{T}(T_{\hat{\mathbf{x}}}+\lambda)^{-1}\right\|^2_{\mathcal{L}(\mathcal{H})} \|g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}\|^2_{\mathcal{H}},$$
$$S_0 \leq \left\|\sqrt{T}(T_{\hat{\mathbf{x}}}+\lambda)^{-1}\right\|^2_{\mathcal{L}(\mathcal{H})} \left\|(T_{\mathbf{x}}-T_{\hat{\mathbf{x}}})f^{\lambda}_{\mathbf{z}}\right\|^2_{\mathcal{H}} \leq \left\|\sqrt{T}(T_{\hat{\mathbf{x}}}+\lambda)^{-1}\right\|^2_{\mathcal{L}(\mathcal{H})} \|T_{\mathbf{x}}-T_{\hat{\mathbf{x}}}\|^2_{\mathcal{L}(\mathcal{H})} \left\|f^{\lambda}_{\mathbf{z}}\right\|^2_{\mathcal{H}}.$$

A.1.10 Proof of the Convergence Rate of the Empirical Mean Embedding

The statement we prove is as follows.[25][9]

Let $\mu_x = \int_{\mathcal{X}} k(\cdot,u)\mathrm{d}x(u)$ denote the mean embedding of distribution $x \in \mathcal{M}_1^+(\mathcal{X})$ to the $H = H(k)$ RKHS determined by kernel k ($\mu_x \in H$), which is assumed to be bounded $k(u,u) \leq B_k$ ($\forall u \in \mathcal{X}$). Let us given N i.i.d. samples from distribution x: x_1, ..., x_N. Let $\mu_{\hat{x}} = \frac{1}{N}\sum_{n=1}^N k(\cdot,x_n) \in H$ be the empirical mean embedding. Then $\mathbb{P}\left(\|\mu_{\hat{x}} - \mu_x\|_H \leq \frac{\sqrt{2B_k}}{\sqrt{N}} + \epsilon\right) \geq 1 - e^{-\frac{\epsilon^2 N}{2B_k}}$, or

$$\|\mu_{\hat{x}_i} - \mu_{x_i}\|_H \leq \frac{\sqrt{2B_k}}{\sqrt{N}} + \frac{\sqrt{2\alpha B_k}}{\sqrt{N}} = \frac{(1+\sqrt{\alpha})\sqrt{2B_k}}{\sqrt{N}}$$

with probability at least $1-e^{-\alpha}$, where $\alpha = \frac{\epsilon^2 N}{2B_k}$.

The proof will make use of the McDiarmid's inequality.

Lemma 1 (**McDiarmid's inequality** [42]). *Let $x_1,\ldots,x_N \in \mathcal{X}$ be independent random variables and function $g \in \mathcal{X}^n \to \mathbb{R}$ be such that $\sup_{u_1,\ldots,u_N,u'_j\in\mathcal{X}} \left|g(u_1,\ldots,u_N) - g(u_1,\ldots,u_{j-1},u'_j,u_{j+1},\ldots,u_N)\right| \leq c_j$ $\forall j = 1,\ldots,N$. Then for all $\epsilon > 0$ $\mathbb{P}\left(g(x_1,\ldots,x_N) - \mathbb{E}\left[g(x_1,\ldots,x_N)\right] \geq \epsilon\right) \leq e^{-\frac{2\epsilon^2}{\sum_{n=1}^N c_n^2}}$.*

Namely, let $\phi(u) = k(\cdot,u)$, and thus $k(u,u) = \|\phi(u)\|^2_H$. Let us define

$$g(S) = \|\mu_{\hat{x}} - \mu_x\|_H = \left\|\frac{1}{N}\sum_{n=1}^N \phi(x_n) - \mu_x\right\|_H,$$

where $S = \{x_1,\ldots,x_N\}$ be the sample set. Define $S' = \{x_1,\ldots,x_{j-1},x'_j,x_{j+1},\ldots,x_N\}$, i.e., let us replace in the sample set x_j with x'_j. Then

$$\begin{aligned}|g(S) - g(S')| &= \left|\left\|\frac{1}{N}\sum_{n=1}^N \phi(x_n) - \mu_x\right\|_H - \left\|\frac{1}{N}\sum_{n=1;n\neq j}^N \phi(x_n) + \frac{1}{N}\phi(x'_j) - \mu_x\right\|_H\right| \\ &\leq \frac{1}{N}\left\|\phi(x_j) - \phi(x'_j)\right\|_H \leq \frac{1}{N}\left(\|\phi(x_j)\|_H + \left\|\phi(x'_j)\right\|_H\right) \leq \frac{1}{N}\left[\sqrt{k(x_j,x_j)} + \sqrt{k\left(x'_j,x'_j\right)}\right] \leq \frac{2\sqrt{B_k}}{N}\end{aligned}$$

based on (i) the reverse and the standard triangle inequality, and (ii) the boundedness of kernel k. By using the McDiarmid's inequality (Lemma 1), we get

$$\mathbb{P}\left(g(S) - \mathbb{E}[g(S)] \geq \epsilon\right) \leq e^{-\frac{2\epsilon^2}{\sum_{n=1}^N \left(\frac{2\sqrt{B_k}}{N}\right)^2}} = e^{-\frac{2\epsilon^2}{N\frac{4B_k}{N^2}}} = e^{-\frac{\epsilon^2 N}{2B_k}},$$

or, in other words

$$1 - e^{-\frac{\epsilon^2 N}{2B_k}} \leq \mathbb{P}\left(g(S) < \mathbb{E}[g(S)] + \epsilon\right) \leq \mathbb{P}\left(g(S) \leq \mathbb{E}[g(S)] + \epsilon\right).$$

[9] In the original result a factor of 2 is missing from the denominator in the exponential function; we correct the proof here.

Considering the $\mathbb{E}[g(S)]$ term: since for a non-negative random variable (a) the $\mathbb{E}(a) = \mathbb{E}(a1) \leq \sqrt{\mathbb{E}(a^2)}\sqrt{\mathbb{E}(1^2)} = \sqrt{\mathbb{E}(a^2)}$ inequality holds due to the CBS, we obtain

$$\mathbb{E}[g(S)] = \mathbb{E}\left[\left\|\frac{1}{N}\sum_{n=1}^{N}\phi(x_n) - \mu_x\right\|_H\right] \leq \sqrt{\mathbb{E}\left[\left\|\frac{1}{N}\sum_{n=1}^{N}\phi(x_n) - \mu_x\right\|_H^2\right]}$$
$$= \sqrt{\mathbb{E}\left[\left\langle\frac{1}{N}\sum_{i=1}^{N}\phi(x_i) - \mu_x, \frac{1}{N}\sum_{j=1}^{N}\phi(x_j) - \mu_x\right\rangle_H\right]} = \sqrt{b+c+d}$$

using that $\|a\|_H^2 = \sqrt{\langle a, a\rangle_H}$. Here,

$$b = \mathbb{E}\left[\frac{1}{N^2}\left(\sum_{i,j=1;i\neq j}^{N}k(x_i,x_j) + \sum_{i=1}^{N}k(x_i,x_i)\right)\right] = \frac{N(N-1)}{N^2}\mathbb{E}_{t\sim x,t'\sim x}k(t,t') + \frac{N}{N^2}\mathbb{E}_{t\sim x}\left[k(t,t)\right],$$
$$c = -\frac{2}{N}\mathbb{E}\left[\left\langle\sum_{i=1}^{N}\phi(x_i), \mu_x\right\rangle_H\right] = -\frac{2N}{N}\mathbb{E}_{t\sim x,t'\sim x}\left[k(t,t')\right],$$
$$d = \mathbb{E}\left[\|\mu_x\|_H^2\right] = \mathbb{E}_{t\sim x,t'\sim x}\left[k(t,t')\right]$$

applying the bilinearity of $\langle\cdot,\cdot\rangle_H$, and the representation property of μ_x. Thus,

$$\sqrt{b+c+d} = \sqrt{\left[\frac{N-1}{N} - 2 + 1\right]\mathbb{E}_{t\sim x,t'\sim x}\left[k(t,t')\right] + \frac{1}{N}\mathbb{E}_{t\sim x}\left[k(t,t)\right]}$$
$$= \sqrt{\frac{1}{N}\left(\mathbb{E}_{t\sim x}\left[k(t,t)\right] - \mathbb{E}_{t\sim x,t'\sim x}\left[k(t,t')\right]\right)} = \frac{\sqrt{\mathbb{E}_{t\sim x}\left[k(t,t)\right] - \mathbb{E}_{t\sim x,t'\sim x}\left[k(t,t')\right]}}{\sqrt{N}}.$$

Since

$$\sqrt{\mathbb{E}_{t\sim x}\left[k(t,t)\right] - \mathbb{E}_{t\sim x,t'\sim x}\left[k(t,t')\right]} \leq \sqrt{\left|\mathbb{E}_{t\sim x}\left[k(t,t)\right]\right| + \left|\mathbb{E}_{t\sim x,t'\sim x}\left[k(t,t')\right]\right|} \leq \sqrt{\mathbb{E}_{t\sim x}\left|k(t,t)\right| + \mathbb{E}_{t\sim x,t'\sim x}\left|k(t,t')\right|},$$

where we applied the triangle inequality, $|k(t,t)| = k(t,t) \leq B_k$ and $|k(t,t')| \leq \sqrt{k(t,t)}\sqrt{k(t',t')}$ (which holds to the CBS), we get $\sqrt{\mathbb{E}_{t\sim x}\left[k(t,t)\right] - \mathbb{E}_{t\sim x,t'\sim x}\left[k(t,t')\right]} \leq \sqrt{B_k + \sqrt{B_k}\sqrt{B_k}} = \sqrt{2B_k}$.

To sum up, we obtained that $\|\mu_x - \mu_{\hat{x}}\|_H \leq \frac{\sqrt{2B_k}}{\sqrt{N}} + \epsilon$ holds with probability at least $1 - e^{-\frac{\epsilon^2 N}{2B_k}}$. This is what we wanted to prove.

A.1.11 Proof of the Bound on $\|g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}\|_{\mathcal{H}}^2$, $\|T_{\mathbf{x}} - T_{\hat{\mathbf{x}}}\|_{\mathcal{L}(\mathcal{H})}^2$, $\|\sqrt{T}(T_{\hat{\mathbf{x}}} + \lambda)^{-1}\|_{\mathcal{L}(\mathcal{H})}^2$, $\|f_{\mathbf{z}}^{\lambda}\|_{\mathcal{H}}^2$

Below, we present the detailed derivations of the upper bounds on $\|g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}\|_{\mathcal{H}}^2$, $\|T_{\mathbf{x}} - T_{\hat{\mathbf{x}}}\|_{\mathcal{L}(\mathcal{H})}^2$, $\|\sqrt{T}(T_{\hat{\mathbf{x}}} + \lambda)^{-1}\|_{\mathcal{L}(\mathcal{H})}^2$ and $\|f_{\mathbf{z}}^{\lambda}\|_{\mathcal{H}}^2$.

- **Bound on $\|g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}\|_{\mathcal{H}}^2$**: By (11), we have $g_{\hat{\mathbf{z}}} - g_{\mathbf{z}} = \frac{1}{l}\sum_{i=1}^{l}\left[K(\cdot,\mu_{\hat{x}_i}) - K(\cdot,\mu_{x_i})\right]y_i$. Applying Eq. (21), the Hölder property of K, the homogenity of norms $\|av\| = |a|\,\|v\|$ $(a \in \mathbb{R})$, assuming that y_i is bounded $(|y_i| \leq C)$, and using (13), we obtain

$$\|g_{\hat{\mathbf{z}}} - g_{\mathbf{z}}\|_{\mathcal{H}}^2 \leq \frac{1}{l^2}l\sum_{i=1}^{l}\|K(\cdot,\mu_{\hat{x}_i}) - K(\cdot,\mu_{x_i})y_i\|_{\mathcal{H}}^2 \leq \frac{L^2}{l}\sum_{i=1}^{l}y_i^2\|\mu_{\hat{x}_i} - \mu_{x_i}\|_H^{2h} \leq \frac{L^2C^2}{l}\sum_{i=1}^{l}\left[\frac{(1+\sqrt{\alpha})\sqrt{2B_k}}{\sqrt{N}}\right]^{2h}$$
$$= L^2C^2\frac{(1+\sqrt{\alpha})^{2h}(2B_k)^h}{N^h}$$

with probability at least $1 - le^{-\alpha}$, based on a union bound.

- **Bound on** $\|T_{\mathbf{x}} - T_{\hat{\mathbf{x}}}\|^2_{\mathcal{L}(\mathcal{H})}$: Using the definition of $T_{\mathbf{x}}$ and $T_{\hat{\mathbf{x}}}$, and (21) with the $\|\cdot\|_{\mathcal{L}(\mathcal{H})}$ operator norm, we get

$$\|T_{\mathbf{x}} - T_{\hat{\mathbf{x}}}\|^2_{\mathcal{L}(\mathcal{H})} \leq \frac{1}{l^2} l \sum_{i=1}^{l} \left\| T_{\mu_{x_i}} - T_{\mu_{\hat{x}_i}} \right\|^2_{\mathcal{L}(\mathcal{H})}. \tag{26}$$

To upper bound the quantities $\|T_{\mu_{x_i}} - T_{\mu_{\hat{x}_i}}\|^2_{\mathcal{L}(\mathcal{H})}$, let us see how T_{μ_u} acts

$$T_{\mu_u}(f) = K(\cdot, \mu_u)\delta_{\mu_u}(f) = K(\cdot, \mu_u) f(\mu_u). \tag{27}$$

If we can prove that

$$\|(T_{\mu_u} - T_{\mu_v})(f)\|_{\mathcal{H}} \leq E \|f\|_{\mathcal{H}}, \tag{28}$$

then this implies $\|T_{\mu_u} - T_{\mu_v}\|_{\mathcal{L}(\mathcal{H})} \leq E$. We continue with the l.h.s. of (28) using (27), (21) with $n = 2$, the homogenity of norms, the reproducing and Hölder property of K:

$$\begin{aligned}
\|(T_{\mu_u} - T_{\mu_v})(f)\|^2_{\mathcal{H}} &= \|K(\cdot, \mu_u)\delta_{\mu_u}(f) - K(\cdot, \mu_v)\delta_{\mu_v}(f)\|^2_{\mathcal{H}} \\
&= \|K(\cdot, \mu_u)\left[\delta_{\mu_u}(f) - \delta_{\mu_v}(f)\right] + \left[K(\cdot, \mu_u) - K(\cdot, \mu_v)\right]\delta_{\mu_v}(f)\|^2_{\mathcal{H}} \\
&\leq 2\left[\|K(\cdot, \mu_u)\left[\delta_{\mu_u}(f) - \delta_{\mu_v}(f)\right]\|^2_{\mathcal{H}} + \|K(\cdot, \mu_u) - K(\cdot, \mu_v)\delta_{\mu_v}(f)\|^2_{\mathcal{H}}\right] \\
&= 2\left[\left[\delta_{\mu_u}(f) - \delta_{\mu_v}(f)\right]^2 \|K(\cdot, \mu_u)\|^2_{\mathcal{H}} + \left[\delta_{\mu_v}(f)\right]^2 \|[K(\cdot, \mu_u) - K(\cdot, \mu_v)]\|^2_{\mathcal{H}}\right] \\
&\leq 2\left[\left[\delta_{\mu_u}(f) - \delta_{\mu_v}(f)\right]^2 K(\mu_u, \mu_u) + L^2 \left[\delta_{\mu_v}(f)\right]^2 \|\mu_u - \mu_v\|^{2h}_H\right].
\end{aligned}$$

By rewriting the first terms, we arrive at

$$\begin{aligned}
\delta_{\mu_u}(f) - \delta_{\mu_v}(f) = \langle f, K(\cdot, \mu_u)\rangle_{\mathcal{H}} - \langle f, K(\cdot, \mu_v)\rangle_{\mathcal{H}} &\leq |\langle f, K(\cdot, \mu_u) - K(\cdot, \mu_v)\rangle_{\mathcal{H}}| \\
&\leq \|f\|_{\mathcal{H}} \|K(\cdot, \mu_u) - K(\cdot, \mu_v)\|_{\mathcal{H}} \leq \|f\|_{\mathcal{H}} L \|\mu_u - \mu_v\|^h_H, \\
\delta_{\mu_v}(f) = \langle f, K(\cdot, \mu_v)\rangle_{\mathcal{H}} \leq |\langle f, K(\cdot, \mu_v)\rangle_{\mathcal{H}}| &\leq \|f\|_{\mathcal{H}} \|K(\cdot, \mu_v)\|_{\mathcal{H}} = \|f\|_{\mathcal{H}} \sqrt{K(\mu_v, \mu_v)},
\end{aligned}$$

where we applied the reproducing and Hölder property of K, the bilinearity of $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ and the CBS inequality. Hence

$$\begin{aligned}
\|(T_{\mu_u} - T_{\mu_v})(f)\|^2_{\mathcal{H}} &\leq 2\left[\|f\|^2_{\mathcal{H}} L^2 \|\mu_u - \mu_v\|^{2h}_H K(\mu_u, \mu_u) + L^2 \|f\|^2_{\mathcal{H}} K(\mu_v, \mu_v) \|\mu_u - \mu_v\|^{2h}_H\right] \\
&= 2L^2 \|f\|^2_{\mathcal{H}} \|\mu_u - \mu_v\|^{2h}_H \left[K(\mu_u, \mu_u) + K(\mu_v, \mu_v)\right].
\end{aligned}$$

Thus

$$E^2 = 2L^2 \|\mu_u - \mu_v\|^{2h}_H \left[K(\mu_u, \mu_u) + K(\mu_v, \mu_v)\right].$$

Exploiting this property in (26), (4), and (13)

$$\begin{aligned}
\|T_{\mathbf{x}} - T_{\hat{\mathbf{x}}}\|^2_{\mathcal{L}(\mathcal{H})} &\leq \frac{2L^2}{l} \sum_{i=1}^{l} \|\mu_{x_i} - \mu_{\hat{x}_i}\|^{2h}_H \left[K(\mu_{x_i}, \mu_{x_i}) + K(\mu_{\hat{x}_i}, \mu_{\hat{x}_i})\right] \leq \frac{4B_K L^2}{l} \sum_{i=1}^{l} \frac{(1+\sqrt{\alpha})^{2h} (2B_k)^h}{N^h} \\
&= \frac{(1+\sqrt{\alpha})^{2h} 2^{h+2} (B_k)^h B_K L^2}{N^h}.
\end{aligned} \tag{29}$$

- **Bound on** $\|\sqrt{T}(T_{\hat{\mathbf{x}}} + \lambda)^{-1}\|^2_{\mathcal{L}(\mathcal{H})}$: First we rewrite $T_{\hat{\mathbf{x}}} + \lambda$,

$$T_{\hat{\mathbf{x}}} + \lambda = (T + \lambda) - (T - T_{\hat{\mathbf{x}}}) = \left[I - (T - T_{\hat{\mathbf{x}}})(T + \lambda)^{-1}\right](T + \lambda).$$

Let us now use the Neumann series of $I - (T - T_{\hat{\mathbf{x}}})(T + \lambda)^{-1}$

$$\sqrt{T}(T_{\hat{\mathbf{x}}} + \lambda)^{-1} = \sqrt{T}(T + \lambda)^{-1} \sum_{n=0}^{\infty} \left[(T - T_{\hat{\mathbf{x}}})(T + \lambda)^{-1}\right]^n$$

to have

$$\begin{aligned}\left\|\sqrt{T}(T_{\hat{\mathbf{x}}}+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})} &= \left\|\sqrt{T}(T+\lambda)^{-1}\sum_{n=0}^{\infty}\left[(T-T_{\hat{\mathbf{x}}})(T+\lambda)^{-1}\right]^n\right\|_{\mathcal{L}(\mathcal{H})}\\ &\leq \left\|\sqrt{T}(T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})}\left\|\sum_{n=0}^{\infty}\left[(T-T_{\hat{\mathbf{x}}})(T+\lambda)^{-1}\right]^n\right\|_{\mathcal{L}(\mathcal{H})}\\ &\leq \left\|\sqrt{T}(T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})}\sum_{n=0}^{\infty}\left\|\left[(T-T_{\hat{\mathbf{x}}})(T+\lambda)^{-1}\right]^n\right\|_{\mathcal{L}(\mathcal{H})}\\ &\leq \left\|\sqrt{T}(T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})}\sum_{n=0}^{\infty}\left\|(T-T_{\hat{\mathbf{x}}})(T+\lambda)^{-1}\right\|^n_{\mathcal{L}(\mathcal{H})},\end{aligned}$$

where $\|AB\|_{\mathcal{L}(\mathcal{H})} \leq \|A\|_{\mathcal{L}(\mathcal{H})}\|B\|_{\mathcal{L}(\mathcal{H})}$ and the triangle inequality was applied. By the spectral theorem, the first term can be bounded as $\|\sqrt{T}(T+\lambda)^{-1}\|_{\mathcal{L}(\mathcal{H})} \leq \frac{1}{2\sqrt{\lambda}}$, whereas for the second term, applying a telescopic trick and a triangle inequality, we get

$$\begin{aligned}\left\|(T-T_{\hat{\mathbf{x}}})(T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})} &= \left\|\left[(T-T_{\mathbf{x}})+(T_{\mathbf{x}}-T_{\hat{\mathbf{x}}})\right](T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})}\\ &\leq \left\|(T-T_{\mathbf{x}})(T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})}+\left\|(T_{\mathbf{x}}-T_{\hat{\mathbf{x}}})(T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})}.\end{aligned}$$

We know that

$$\boldsymbol{\Theta}(\lambda,\mathbf{z}) := \|(T-T_{\mathbf{x}})(T+\lambda)^{-1}\|_{\mathcal{L}(\mathcal{H})} \leq \frac{1}{2} \tag{30}$$

with probability at least $1-\frac{\eta}{3}$ [5]. Considering the second term, using (29) and $\|(T+\lambda)^{-1}\|_{\mathcal{L}(\mathcal{H})} \leq \frac{1}{\lambda}$ (by the spectral theorem),

$$\left\|(T_{\mathbf{x}}-T_{\hat{\mathbf{x}}})(T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})} \leq \|T_{\mathbf{x}}-T_{\hat{\mathbf{x}}}\|_{\mathcal{L}(\mathcal{H})}\left\|(T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})} \leq \frac{(1+\sqrt{\alpha})^h 2^{\frac{h}{2}+1}(B_k)^{\frac{h}{2}}(B_K)^{\frac{1}{2}}L}{N^{\frac{h}{2}}}\frac{1}{\lambda}.$$

For fixed λ, the value of N can be chosen such that

$$\begin{aligned}&\frac{(1+\sqrt{\alpha})^h 2^{\frac{h}{2}+1}(B_k)^{\frac{h}{2}}(B_K)^{\frac{1}{2}}L}{N^{\frac{h}{2}}}\frac{1}{\lambda} \leq \frac{1}{4} \Leftrightarrow \frac{(1+\sqrt{\alpha})^h 2^{\frac{h}{2}+3}(B_k)^{\frac{h}{2}}(B_K)^{\frac{1}{2}}L}{\lambda} \leq N^{\frac{h}{2}} \Leftrightarrow\\ &\frac{(1+\sqrt{\alpha})^2 2^{\frac{h+6}{h}}B_k(B_K)^{\frac{1}{h}}L^{\frac{2}{h}}}{\lambda^{\frac{2}{h}}} \leq N.\end{aligned} \tag{31}$$

In this case $\left\|(T-T_{\hat{\mathbf{x}}})(T+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})} \leq \frac{3}{4}$ (the Neumann series trick is legitimate) and

$$\left\|\sqrt{T}(T_{\hat{\mathbf{x}}}+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})} \leq \frac{1}{2\sqrt{\lambda}}\frac{1}{1-\frac{3}{4}} \leq \frac{2}{\sqrt{\lambda}}. \tag{32}$$

- **Bound on** $\|f^{\lambda}_{\mathbf{z}}\|^2_{\mathcal{H}}$: Using the explicit form of $f^{\lambda}_{\mathbf{z}}$ [(9)], (25), the positivity of $T_{\mathbf{x}}$ $\left[\Rightarrow \left\|(T_{\mathbf{x}}+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})} \leq \frac{1}{\lambda}\right]$, the homogenity of norms, Eq. (21), the boundedness assumption on y_i ($|y_i| \leq C$), the reproducing property and the boundedness of K [Eq. (4)], we get

$$\left\|f^{\lambda}_{\mathbf{z}}\right\|_{\mathcal{H}} \leq \left\|(T_{\mathbf{x}}+\lambda)^{-1}\right\|_{\mathcal{L}(\mathcal{H})}\|g_{\mathbf{z}}\|_{\mathcal{H}} \leq \frac{1}{\lambda}\|g_{\mathbf{z}}\|_{\mathcal{H}},$$

where

$$\|g_{\mathbf{z}}\|^2_{\mathcal{H}} \leq \frac{1}{l^2}l\sum_{i=1}^{l}\|K(\cdot,\mu_{x_i})y_i\|^2_{\mathcal{H}} \leq \frac{1}{l}\sum_{i=1}^{l}C^2\|K(\cdot,\mu_{x_i})\|^2_{\mathcal{H}} = \frac{1}{l}\sum_{i=1}^{l}C^2K(\mu_{x_i},\mu_{x_i}) \leq \frac{1}{l}\sum_{i=1}^{l}C^2B_K = C^2B_K.$$

Thus, we have obtained that

$$\left\|f^{\lambda}_{\mathbf{z}}\right\|^2_{\mathcal{H}} \leq \frac{1}{\lambda^2}C^2B_K. \tag{33}$$

A.1.12 Final Step of the Proof (Union Bound)

Until now, we obtained that if

1. the sample number N satisfies Eq. (31),
2. (13) holds for $\forall i = 1, \dots, l$ (which has probability at least $1 - le^{-\alpha} = 1 - e^{-[\alpha - \log(l)]} = 1 - e^{-\delta}$ applying a union bound argument; $\alpha = \log(l) + \delta$), and
3. $\mathbf{\Theta}(\lambda, \mathbf{z}) \leq \frac{1}{2}$ is fulfilled [see Eq. (30)], then

$$S_{-1} + S_0 \leq \frac{4}{\lambda}\left[L^2 C^2 \frac{(1+\sqrt{\alpha})^{2h}(2B_k)^h}{N^h} + \frac{(1+\sqrt{\alpha})^{2h} 2^{h+2}(B_k)^h B_K L^2}{N^h}\frac{C^2 B_K}{\lambda^2}\right]$$
$$= \frac{4L^2C^2(1+\sqrt{\alpha})^{2h}(2B_k)^h}{\lambda N^h}\left[1 + \frac{4(B_K)^2}{\lambda^2}\right].$$

By taking into account [5]'s bounds for S_1 and S_2

$$S_1 \leq 32\log^2\left(\frac{6}{\eta}\right)\left[\frac{B_K M^2}{l^2\lambda} + \frac{\Sigma^2 \mathcal{N}(\lambda)}{l}\right], \qquad S_2 \leq 8\log^2\left(\frac{6}{\eta}\right)\left[\frac{4B_K^2 \mathcal{B}(\lambda)}{l^2\lambda} + \frac{B_K \mathcal{A}(\lambda)}{l\lambda}\right],$$

plugging all the expressions to (24), we obtain Theorem 4 via a union bound.

A.1.13 Proof of Consequence 2

Since constant multipliers do not matter in the orders of rates, we discard them in the (in)equalities below. Our goal is to choose $\lambda = \lambda_{l,N}$ such that

- $\lim_{l,N\to\infty} \lambda_{l,N} = 0$, and
- in Theorem 4: (i') $\frac{\log(l)}{\lambda^{\frac{2}{h}}} \leq N$, (i) $l\lambda^{\frac{b+1}{b}} \geq 1$,[10] and (ii) $r(l, N, \lambda) = \frac{\log^h(l)}{N^h\lambda^3} + \lambda^c + \frac{\lambda^{c-2}}{l^2} + \frac{\lambda^{c-1}}{l} + \frac{1}{l^2\lambda} + \frac{1}{l\lambda^{\frac{1}{b}}} \to 0$.

In $r(l, N, \lambda)$ we will require that the first term goes to zero $\left[\frac{\log^h(l)}{N^h\lambda^3} \to 0\right]$, which implies $\frac{\log(l)}{N\lambda^{\frac{2}{h}}} \to 0$ and hence $\frac{\log(l)}{N\lambda^{\frac{2}{h}}} \to 0$. Thus constraint (i') can be discarded, and our goal is to fulfill (i)-(ii). Since

1. $2 - c \leq 1$ ($\Leftrightarrow 1 \leq c$), $\frac{1}{l^2\lambda^{2-c}} = \frac{\lambda^{c-2}}{l^2} \leq \frac{1}{l^2\lambda}$ (in order), and
2. $c - 1 \geq 0$ ($\Leftrightarrow 1 \leq c$), $\frac{\lambda^{c-1}}{l} \leq \frac{1}{l\lambda^{\frac{1}{b}}}$ (in order)

condition (i)-(ii) reduces to

$$r(l, N, \lambda) = \frac{\log^h(l)}{N^h\lambda^3} + \lambda^c + \frac{1}{l^2\lambda} + \frac{1}{l\lambda^{\frac{1}{b}}} \to 0, \text{ subject to } l\lambda^{\frac{b+1}{b}} \geq 1. \tag{34}$$

Our goal is to study the behavior of this quantity in terms of the (l, N, λ) triplet; $1 < b$, $c \in [1, 2]$, $h \in (0, 1]$. To do so, we

1. choose λ such a way that two terms match in order (and $\lambda = \lambda_{l,N} \to 0$);
2. setting $l = N^a$ ($a > 0$) we examine under what conditions (i)-(ii) the convergence of r to 0 holds with the constraint $l\lambda^{\frac{b+1}{b}} \geq 1$ satisfied, (iii) are the matched terms also dominant, i.e., give the convergence rate.

We carry out the computation for all the $\binom{4}{2} = 6$ pairs in Eq. (34). Below we give the derivation of the results summarized in Table 2.

- $\boxed{1} = \boxed{2}$ in Eq. (34) [i.e., the first and second terms are equal in Eq. (34)]:

[10] $\mathcal{N}(\lambda)$ can be upper bounded by (constant multipliers are discarded) $\lambda^{-\frac{1}{b}}$ [5]. Using this upper bound in the l constraint of Theorem 4 we get $l \geq \frac{\lambda^{-\frac{1}{b}}}{\lambda} \Leftrightarrow l\lambda^{\frac{1}{b}+1=\frac{b+1}{b}} \geq 1$.

– (i)-(ii): Exploiting $\frac{h}{c+3} > 0$ in the λ choice, we get

$$\frac{\log^h(l)}{N^h\lambda^3} = \lambda^c \Leftrightarrow \left[\frac{\log(l)}{N}\right]^h = \lambda^{c+3} \Leftrightarrow \left[\frac{\log(l)}{N}\right]^{\frac{h}{c+3}} = \lambda \to 0, \text{ if } \frac{\log(l)}{N} \to 0.$$

$$r(l,N) = \left[\frac{\log(l)}{N}\right]^{\frac{hc}{c+3}} + \frac{1}{l^2\left[\frac{\log(l)}{N}\right]^{\frac{h}{c+3}}} + \frac{1}{l\left[\frac{\log(l)}{N}\right]^{\frac{h}{b(c+3)}}}.$$

$$\begin{aligned} r(N) &= \left[\frac{\log(N)}{N}\right]^{\frac{hc}{c+3}} + \frac{1}{N^{2a}\left[\frac{\log(N)}{N}\right]^{\frac{h}{c+3}}} + \frac{1}{N^a\left[\frac{\log(N)}{N}\right]^{\frac{h}{b(c+3)}}} \\ &= \left[\frac{\log(N)}{N}\right]^{\frac{hc}{c+3}} + \frac{N^{\frac{h}{c+3}}}{N^{2a}\log^{\frac{h}{c+3}}(N)} + \frac{N^{\frac{h}{b(c+3)}}}{N^a\log^{\frac{h}{b(c+3)}}(N)}. \end{aligned} \tag{35}$$

Here,

* (ii): $r(N) \to 0$ if
  - $\boxed{1} \to 0$: [i.e., the first term goes to zero in Eq. (35)]; no constraint using that $\frac{hc}{c+3} > 0$.
  - $\boxed{2} \to 0$: $2a \geq \frac{h}{c+3}$ [$\Leftarrow \frac{h}{c+3} > 0$].
  - $\boxed{3} \to 0$: $a \geq \frac{h}{b(c+3)}$ [$\Leftarrow \frac{h}{b(c+3)} > 0$],

  i.e., $a \geq \max\left(\frac{h}{2(c+3)}, \frac{h}{b(c+3)}\right) = \frac{h}{(c+3)\min(2,b)}$.
* (i): We require $N^a\left(\left[\frac{\log(N)}{N}\right]^{\frac{h}{c+3}}\right)^{\frac{b+1}{b}} \geq 1 \Leftrightarrow \frac{\log^{\frac{h}{c+3}\frac{b+1}{b}}(N)}{N^{\frac{h}{c+3}\frac{b+1}{b}-a}} \geq 1$. Since $\frac{h}{c+3}\frac{b+1}{b} > 0$, it is sufficient to have $\frac{h}{c+3}\frac{b+1}{b} - a \leq 0 \Leftrightarrow \frac{h(b+1)}{(c+3)b} \leq a$.

To sum up, for (i)-(ii) we got $a \geq \max\left(\frac{h}{(c+3)\min(2,b)}, \frac{h(b+1)}{(c+3)b}\right)$.

– (iii):
* (i): $\frac{h(b+1)}{(c+3)b} \leq a$.
* $\boxed{1} \to 0$: no constraint.
* $\boxed{1} \geq \boxed{2}$ [i.e., the first term dominates the second one in Eq. (35)]: $\left[\frac{\log(N)}{N}\right]^{\frac{hc}{c+3}} \geq \frac{N^{\frac{h}{c+3}}}{N^{2a}\log^{\frac{h}{c+3}}(N)} \Leftrightarrow \log^{\frac{hc}{c+3}+\frac{h}{c+3}}(N) \geq N^{\frac{hc}{c+3}+\frac{h}{c+3}-2a}$. Thus, since $\frac{h(c+1)}{c+3} > 0$ we need $\frac{h(c+1)}{c+3} - 2a \leq 0$, i.e., $\frac{h(c+1)}{2(c+3)} \leq a$.
* $\boxed{1} \geq \boxed{3}$ [i.e., the first term dominates the third one in Eq. (35)]: $\left[\frac{\log(N)}{N}\right]^{\frac{hc}{c+3}} \geq \frac{N^{\frac{h}{b(c+3)}}}{N^a\log^{\frac{h}{b(c+3)}}(N)} \Leftrightarrow \log^{\frac{hc}{c+3}+\frac{h}{b(c+3)}}(N) \geq N^{\frac{h}{b(c+3)}+\frac{hc}{c+3}-a}$. Since $\frac{hc}{c+3} + \frac{h}{b(c+3)} > 0$ we require $\frac{h}{b(c+3)} + \frac{hc}{c+3} - a \leq 0$, i.e., $\frac{h}{b(c+3)} + \frac{hc}{c+3} \leq a$.

To sum up, the obtained condition for a is $\max\left(\frac{h}{b(c+3)} + \frac{hc}{c+3}, \frac{h(c+1)}{2(c+3)}\right) = \frac{h\max\left(\frac{1}{b}+c, \frac{c+1}{2}\right)}{c+3} \leq a$. Since $\frac{1}{b} + c \geq \frac{c+1}{2} \Leftrightarrow \frac{1}{b} + \frac{c}{2} \geq \frac{1}{2}$[$\Leftarrow c \geq 1, b > 0$], we got

$$\max\left(\frac{h\left(\frac{1}{b}+c\right)}{c+3}, \frac{h(b+1)}{(c+3)b}\right) \leq a, \qquad r(N) = \left[\frac{\log(N)}{N}\right]^{\frac{hc}{c+3}} \to 0.$$

- $\boxed{1} = \boxed{3}$ in Eq. (34):

– (i)-(ii): Using in the λ choice that $\frac{h}{2}>0$, we obtain that

$$\frac{\log^h(l)}{N^h\lambda^3}=\frac{1}{l^2\lambda}\Leftrightarrow\frac{l^2\log^h(l)}{N^h}=\lambda^2\Leftrightarrow\frac{l\log^{\frac{h}{2}}(l)}{N^{\frac{h}{2}}}=\lambda\to 0,\text{ if } a<\frac{h}{2}\text{ in } l=N^a.$$

$$r(l,N)=\left[\frac{l\log^{\frac{h}{2}}(l)}{N^{\frac{h}{2}}}\right]^c+\frac{1}{l^2\frac{l\log^{\frac{h}{2}}(l)}{N^{\frac{h}{2}}}}+\frac{1}{l\left[\frac{l\log^{\frac{h}{2}}(l)}{N^{\frac{h}{2}}}\right]^{\frac{1}{b}}}.$$

$$r(N)=N^{ac-\frac{hc}{2}}\log^{\frac{hc}{2}}(N)+\frac{1}{N^{3a-\frac{h}{2}}\log^{\frac{h}{2}}(N)}+\frac{1}{N^{a+\frac{a}{b}-\frac{h}{2b}}\log^{\frac{h}{2b}}(N)}.$$

Here,

∗ (ii): $r(N)\to 0$ if
  · $\boxed{1}\to 0$: $ac-\frac{hc}{2}=c\left(a-\frac{h}{2}\right)<0$ [$\Leftarrow\frac{hc}{2}>0$], i.e., $a<\frac{h}{2}$ using that $c>0$.
  · $\boxed{2}\to 0$: $3a-\frac{h}{2}\geq 0$ [$\Leftarrow\frac{h}{2}>0$], i.e., $\frac{h}{6}\leq a$.
  · $\boxed{3}\to 0$: $a+\frac{a}{b}-\frac{h}{2b}\geq 0$ [$\Leftarrow\frac{h}{2b}>0$], i.e., $\frac{h}{2b\left(1+\frac{1}{b}\right)}=\frac{h}{2b\frac{b+1}{b}}=\frac{h}{2(b+1)}\leq a$ exploiting that $1+\frac{1}{b}>0$.

  In other words, the requirement is $\max\left(\frac{h}{6},\frac{h}{2(b+1)}\right)\leq a<\frac{h}{2}$.

∗ (i): $N^a\left[\frac{N^a\log^{\frac{h}{2}}(N)}{N^{\frac{h}{2}}}\right]^{\frac{b+1}{b}}\geq 1\Leftrightarrow\frac{\log^{\frac{h}{2}\frac{b+1}{b}}(N)}{N^{\frac{h}{2}\frac{b+1}{b}-a-a\frac{b+1}{b}}}\geq 1$. Since $\frac{h}{2}\frac{b+1}{b}>0$ it is enough to have $\frac{h}{2}\frac{b+1}{b}-a-a\frac{b+1}{b}\leq 0\Leftrightarrow\frac{h}{2}\frac{b+1}{b}\leq a\left(1+\frac{b+1}{b}\right)=a\frac{2b+1}{b}\Leftrightarrow\frac{h}{2}\frac{b+1}{2b+1}\leq a$ using that $2b+1>0$, $b>0$ [$\Leftarrow b>1$].

To sum up, for (i)-(ii) we obtained $\max\left(\frac{h}{6},\frac{h}{2(b+1)},\frac{h}{2}\frac{b+1}{2b+1}\right)\leq a<\frac{h}{2}$.

– (iii):

∗ (i): $\frac{h}{2}\frac{b+1}{2b+1}\leq a$

∗ $\boxed{2}\to 0$: $\frac{h}{6}\leq a$.

∗ $\boxed{2}\geq\boxed{1}$: $\frac{1}{N^{3a-\frac{h}{2}}\log^{\frac{h}{2}}(N)}\geq N^{ac-\frac{hc}{2}}\log^{\frac{hc}{2}}(N)\Leftrightarrow N^{\frac{h}{2}-3a+\frac{hc}{2}-ac}\geq\log^{\frac{h(c+1)}{2}}(N)$. Thus, since $\frac{h(c+1)}{2}>0$ we need $\frac{h}{2}-3a+\frac{hc}{2}-ac>0$, i.e., $\frac{h(c+1)}{2(c+3)}=\frac{h(c+3-2)}{2(c+3)}=\frac{h}{2}-\frac{h}{c+3}>a$, using that $c+3>0$.

∗ $\boxed{2}\geq\boxed{3}$: $\frac{1}{N^{3a-\frac{h}{2}}\log^{\frac{h}{2}}(N)}\geq\frac{1}{N^{a+\frac{a}{b}-\frac{h}{2b}}\log^{\frac{h}{2b}}(N)}\Leftrightarrow N^{a+\frac{a}{b}-\frac{h}{2b}+\frac{h}{2}-3a}\geq\log^{\frac{h}{2}-\frac{h}{2b}}(N)$. Since $\frac{h}{2}-\frac{h}{2b}=\frac{h}{2}\left(1-\frac{1}{b}\right)>0$ using that $h>0$ and $b>1$, we need $a+\frac{a}{b}-\frac{h}{2b}+\frac{h}{2}-3a>0$, i.e., $a\left(1+\frac{1}{b}-3\right)>\frac{h}{2}\left(\frac{1}{b}-1\right)\Leftrightarrow a\left(\frac{1}{b}-2\right)>\frac{h}{2}\left(\frac{1}{b}-1\right)$. Using that $b>1$, $0>\frac{1}{b}-1>\frac{1}{b}-2$; hence $a<\frac{\frac{h}{2}\left(\frac{1}{b}-1\right)}{\frac{1}{b}-2}$.

To sum up, we got

$$\max\left(\frac{h}{6},\frac{h}{2}\frac{b+1}{2b+1}\right)\leq a<\min\left(\frac{h}{2}-\frac{h}{c+3},\frac{\frac{h}{2}\left(\frac{1}{b}-1\right)}{\frac{1}{b}-2}\right)\qquad r(N)=\frac{1}{N^{3a-\frac{h}{2}}\log^{\frac{h}{2}}(N)}\to 0.$$

- $\boxed{1}=\boxed{4}$ in Eq. (34):

– (i)-(ii): Using in the λ choice that $\frac{b}{3b-1}>0$, we get

$$\frac{\log^h(l)}{N^h\lambda^3}=\frac{1}{l\lambda^{\frac{1}{b}}}\Leftrightarrow\frac{l\log^h(l)}{N^h}=\lambda^{3-\frac{1}{b}=\frac{3b-1}{b}}\Leftrightarrow\left[\frac{l\log^h(l)}{N^h}\right]^{\frac{b}{3b-1}}=\lambda\to 0,\text{ if } h>a\text{ in } l=N^a.$$

$$r(l,N)=\left[\frac{l\log^h(l)}{N^h}\right]^{\frac{bc}{3b-1}}+\frac{1}{l^2\left[\frac{l\log^h(l)}{N^h}\right]^{\frac{b}{3b-1}}}+\frac{1}{l\left[\frac{l\log^h(l)}{N^h}\right]^{\frac{1}{3b-1}}}.$$

$$r(N)=\left[\frac{\log^h(N)}{N^{h-a}}\right]^{\frac{bc}{3b-1}}+\frac{1}{N^{2a+\frac{ab}{3b-1}-\frac{hb}{3b-1}}\log^{\frac{hb}{3b-1}}(N)}+\frac{1}{N^{a+\frac{a}{3b-1}-\frac{h}{3b-1}}\log^{\frac{h}{3b-1}}(N)}.$$

Here,

* (ii): $r(N)\to 0$, if
  - $\boxed{1}\to 0$: $h-a>0$ using that $h>0$ and $\frac{bc}{3b-1}>0$, i.e., $a<h$,
  - $\boxed{2}\to 0$: $2a+\frac{ab}{3b-1}-\frac{hb}{3b-1}\geq 0$ [using that $\frac{hb}{3b-1}>0$]. In other words, $a\left(2+\frac{b}{3b-1}\right)\geq\frac{hb}{3b-1}\Leftrightarrow a\geq\frac{\frac{hb}{3b-1}}{\left(2+\frac{b}{3b-1}\right)}=\frac{hb}{3b-1}\frac{3b-1}{6b-2+b}=\frac{hb}{7b-2}$ using that $\left(2+\frac{b}{3b-1}\right)>0$.
  - $\boxed{3}\to 0$: $a+\frac{a}{3b-1}-\frac{h}{3b-1}\geq 0$ [using that $\frac{h}{3b-1}>0$], i.e., $a\left(1+\frac{1}{3b-1}\right)\geq\frac{h}{3b-1}\Leftrightarrow a\geq\frac{\frac{h}{3b-1}}{1+\frac{1}{3b-1}}=\frac{h}{3b-1}\frac{3b-1}{3b-1+1}=\frac{h}{3b}$ making use of $\left(1+\frac{1}{3b-1}\right)>0$.

  Thus, we need $\max\left(\frac{hb}{7b-2},\frac{h}{3b}\right)\leq a<h$.
* (i): $N^a\left(\left[\frac{N^a\log^h(N)}{N^h}\right]^{\frac{b}{3b-1}}\right)^{\frac{b+1}{b}}\geq 1\Leftrightarrow\frac{\log^{\frac{h(b+1)}{3b-1}}(N)}{N^{\frac{h(b+1)}{3b-1}-a-a\frac{b+1}{3b-1}}}\leq 1$. Since $\frac{h(b+1)}{3b-1}>0$, it is sufficient $\frac{h(b+1)}{3b-1}-a-a\frac{b+1}{3b-1}\leq 0\Leftrightarrow\frac{h(b+1)}{3b-1}\leq a\left(1+\frac{b+1}{3b-1}\right)=a\frac{3b-1+b+1}{3b-1}=a\frac{4b}{3b-1}\Leftrightarrow\frac{h(b+1)}{4b}\leq a$, where we used that $4b>0$, $3b-1>0$ [$\Leftarrow b>1$].

To sum up, for (i)-(ii) we received $\max\left(\frac{hb}{7b-2},\frac{h}{3b},\frac{h(b+1)}{4b}\right)\leq a<h$.

– (iii):
* (i): $\frac{h(b+1)}{4b}\leq a$.
* $\boxed{3}\to 0$: $a\geq\frac{h}{3b}$.
* $\boxed{3}\geq\boxed{1}$: $\frac{1}{N^{a+\frac{a}{3b-1}-\frac{h}{3b-1}}\log^{\frac{h}{3b-1}}(N)}\geq\left[\frac{\log^h(N)}{N^{h-a}}\right]^{\frac{bc}{3b-1}}\Leftrightarrow N^{\frac{(h-a)bc}{3b-1}-a-\frac{a}{3b-1}+\frac{h}{3b-1}}\geq\log^{\frac{h(bc+1)}{3b-1}}(N)$.
  Since $\frac{h(bc+1)}{3b-1}>0$, we need $\frac{(h-a)bc}{3b-1}-a-\frac{a}{3b-1}+\frac{h}{3b-1}>0\Leftrightarrow\frac{h(bc+1)}{3b-1}>a\left(\frac{bc}{3b-1}+1+\frac{1}{3b-1}\right)\Leftrightarrow\frac{h(bc+1)}{3b-1}>a\left(1+\frac{bc+1}{3b-1}\right)\Leftrightarrow\frac{h(bc+1)}{3b-1}>a\frac{3b-1+bc+1}{3b-1}\Leftrightarrow\frac{h(bc+1)}{3b-1}>a\frac{3b+bc}{3b-1}\Leftrightarrow\frac{h(bc+1)}{3b+bc}>a$
  using at the last step that $3b-1>0$ and $3b+bc>0$.
* $\boxed{3}\geq\boxed{2}$: $\frac{1}{N^{a+\frac{a}{3b-1}-\frac{h}{3b-1}}\log^{\frac{h}{3b-1}}(N)}\geq\frac{1}{N^{2a+\frac{ab}{3b-1}-\frac{hb}{3b-1}}\log^{\frac{hb}{3b-1}}(N)}\Leftrightarrow$
  $\log^{\frac{h(b-1)}{3b-1}}(N)\geq N^{-2a-\frac{ab}{3b-1}+\frac{hb}{3b-1}+a+\frac{a}{3b-1}-\frac{h}{3b-1}}$. Since $\frac{h(b-1)}{3b-1}>0$, we require that $-2a-\frac{ab}{3b-1}+\frac{hb}{3b-1}+a+\frac{a}{3b-1}-\frac{h}{3b-1}\leq 0\Leftrightarrow\frac{h(b-1)}{3b-1}\leq a\left(1+\frac{b-1}{3b-1}\right)\Leftrightarrow\frac{h(b-1)}{3b-1}\leq a\frac{3b-1+b-1}{3b-1}\Leftrightarrow\frac{h(b-1)}{4b-2}\leq a$ using that $3b-1>0$ and $4b-2>0$.

To sum up, we obtained that

$$\max\left(\frac{h(b-1)}{4b-2},\frac{h}{3b},\frac{h(b+1)}{4b}\right)\leq a<\frac{h(bc+1)}{3b+bc},\qquad r(N)=\frac{1}{N^{a+\frac{a}{3b-1}-\frac{h}{3b-1}}\log^{\frac{h}{3b-1}}(N)}\to 0.$$

- $\boxed{2}=\boxed{3}$ in Eq. (34):

– (i)-(ii):

$$\lambda^c=\frac{1}{l^2\lambda}\Leftrightarrow\lambda^{c+1}=\frac{1}{l^2}\Leftrightarrow\lambda=\frac{1}{l^{\frac{2}{c+1}}}\to 0,\ \text{if } l\to\infty.\quad[\Leftarrow\frac{2}{c+1}>0]$$

$$r(l,N)=\frac{l^{\frac{6}{c+1}}\log^h(l)}{N^h}+\frac{1}{l^{\frac{2c}{c+1}}}+\frac{l^{\frac{2}{b(c+1)}}}{l}\Rightarrow r(N)=\frac{\log^h(N)}{N^{h-\frac{6a}{c+1}}}+\frac{1}{N^{\frac{2ac}{c+1}}}+\frac{1}{N^{a\left(1-\frac{2}{b(c+1)}\right)}}.$$

Here,
* (ii): $r(N)\to 0$ if
  - $\boxed{1}\to 0$: $h-\frac{6a}{c+1}>0$ since $h>0$, i.e., $a<\frac{h(c+1)}{6}$ using that $c+1>0$.
  - $\boxed{2}\to 0$: $\frac{2ac}{c+1}>0$ – this condition is satisfied by our assumptions ($a>0$, $c>0$).
  - $\boxed{3}\to 0$: $a\left(1-\frac{2}{b(c+1)}\right)>0$. Using that $a>0$, $b>0$, $c+1>0$ this requirement is $1>\frac{2}{b(c+1)}\Leftrightarrow b(c+1)>2[\Leftarrow b>1,c\geq 1]$.

  Thus, we need $a<\frac{h(c+1)}{6}$.
* (i): $N^a\left(\frac{1}{N^{\frac{2a}{c+1}}}\right)^{\frac{b+1}{b}}\geq 1\Leftrightarrow N^{a-\frac{2a(b+1)}{(c+1)b}}\geq 1$. Thus it is enough to satisfy $a-\frac{2a(b+1)}{(c+1)b}>0\Leftrightarrow 1>\frac{2(b+1)}{(c+1)b}$, where we used that $a>0$.

To sum up, for (i)-(ii) we obtained $a < \frac{h(c+1)}{6}$, $1 > \frac{2(b+1)}{(c+1)b}$.

– (iii):

∗ (i): $1 > \frac{2(b+1)}{(c+1)b}$.

∗ $\boxed{2} \to 0$: no constraint.

∗ $\boxed{2} \geq \boxed{1}$: $\frac{1}{N^{\frac{2ac}{c+1}}} \geq \frac{\log^h(N)}{N^{h-\frac{6a}{c+1}}} \Leftrightarrow N^{h-\frac{6a}{c+1}-\frac{2ac}{c+1}} \geq \log^h(N)$. Thus, since $h > 0$ we require that $h - \frac{6a}{c+1} - \frac{2ac}{c+1} > 0 \Leftrightarrow h > a\frac{6+2c}{c+1} \Leftrightarrow \frac{h(c+1)}{6+2c} > a$, where the $6 + 2c > 0$, $c + 1 > 0$ relations were exploited [$\Leftarrow c \geq 1$].

∗ $\boxed{2} \geq \boxed{3}$: $\frac{1}{N^{\frac{2ac}{c+1}}} \geq \frac{1}{N^{a\left(1-\frac{2}{b(c+1)}\right)}} \Leftrightarrow N^{a\left(1-\frac{2}{b(c+1)}\right)-\frac{2ac}{c+1}} \geq 1$. Hence, by $a > 0$ and $c + 1 > 0$ we need $a\left(1 - \frac{2}{b(c+1)}\right) - \frac{2ac}{c+1} > 0 \Leftrightarrow a\frac{b(c+1)-2}{b(c+1)} > \frac{2ac}{c+1} \Leftrightarrow b(c+1) - 2 > 2bc \Leftrightarrow b - 2 > bc \Leftrightarrow -2 > b(c-1)$. Since $b > 0$ and $c \geq 1$, $b(c-1) \geq 0$; thus, this condition is never satisfied.

- $\boxed{2} = \boxed{4}$ in Eq. (34):

– (i)-(ii):

$$\lambda^c = \frac{1}{l\lambda^{\frac{1}{b}}} \Leftrightarrow \lambda^{c+\frac{1}{b}=\frac{cb+1}{b}} = \frac{1}{l} \Leftrightarrow \lambda = \frac{1}{l^{\frac{b}{bc+1}}} \to 0, \text{ if } l \to \infty \quad [\Leftarrow \frac{b}{bc+1} > 0].$$

$$r(l,N) = \frac{l^{\frac{3b}{bc+1}}\log^h(l)}{N^h} + \frac{1}{l^{\frac{bc}{bc+1}}} + \frac{l^{\frac{b}{bc+1}}}{l^2} \Rightarrow r(N) = \frac{\log^h(N)}{N^{h-\frac{3ab}{bc+1}}} + \frac{1}{N^{\frac{abc}{bc+1}}} + \frac{1}{N^{2a-\frac{ab}{bc+1}}}.$$

Here,

∗ (ii): $r(N) \to 0$, if

· $\boxed{1} \to 0$: Since $h > 0$ we get $h - \frac{3ab}{bc+1} > 0$, i.e., $\frac{h(bc+1)}{3b} > a$ using that $b > 0$, $bc + 1 > 0$.

· $\boxed{2} \to 0$: $\frac{abc}{bc+1} > 0$ – the second condition is satisfied by our assumptions ($a > 0$, $b > 0$, $c > 0$).

· $\boxed{3} \to 0$: $2a - \frac{ab}{bc+1} > 0$. Making use of the positivity of a and $bc + 1$, this requirement is equivalent to $2 > \frac{b}{bc+1} \Leftrightarrow 2bc + 2 > b \Leftrightarrow 2 > b(1 - 2c)$, which holds since $b(1 - 2c) < 0$.

Thus, we need $\frac{h(bc+1)}{3b} > a$.

∗ (i): $N^a\left(\frac{1}{N^{\frac{ab}{bc+1}}}\right)^{\frac{b+1}{b}} \geq 1 \Leftrightarrow N^{a-\frac{a(b+1)}{bc+1}} \geq 1$. Thus it is sufficient to have $a - \frac{a(b+1)}{bc+1} > 0 \Leftrightarrow 1 > \frac{b+1}{bc+1}$, using $a > 0$.

To sum up, for (i)-(ii) we got $\frac{h(bc+1)}{3b} > a$, $1 > \frac{b+1}{bc+1}$.

– (iii):

∗ (i): $1 > \frac{b+1}{bc+1}$.

∗ $\boxed{2} \to 0$: no constraint.

∗ $\boxed{2} \geq \boxed{1}$: $\frac{1}{N^{\frac{abc}{bc+1}}} \geq \frac{\log^h(N)}{N^{h-\frac{3ab}{bc+1}}} \Leftrightarrow N^{h-\frac{3ab}{bc+1}-\frac{abc}{bc+1}} \geq \log^h(N)$. Since $h > 0$, this holds if $h - \frac{3ab}{bc+1} - \frac{abc}{bc+1} > 0 \Leftrightarrow h > a\frac{3b+bc}{bc+1} \Leftrightarrow \frac{h(bc+1)}{3b+bc} > a$, exploiting that $3b + bc > 0$, $bc + 1 > 0$.

∗ $\boxed{2} \geq \boxed{3}$: $\frac{1}{N^{\frac{abc}{bc+1}}} \geq \frac{1}{N^{2a-\frac{ab}{bc+1}}} \Leftrightarrow N^{2a-\frac{ab}{bc+1}-\frac{abc}{bc+1}} \geq 1$. Hence, since $a > 0$ and $bc + 1 > 0$ we have $2a - \frac{ab}{bc+1} - \frac{abc}{bc+1} > 0 \Leftrightarrow 2 > \frac{b+bc}{bc+1} \Leftrightarrow 2bc + 2 > b + bc \Leftrightarrow bc + 2 > b \Leftrightarrow 2 > b(1 - c)$. This holds since $b(1 - c) \leq 0$.

Thus, we got

$$\frac{h(bc+1)}{3b+bc} > a, \qquad 1 > \frac{b+1}{bc+1} \qquad r(N) = \frac{1}{N^{\frac{abc}{bc+1}}} \to 0.$$

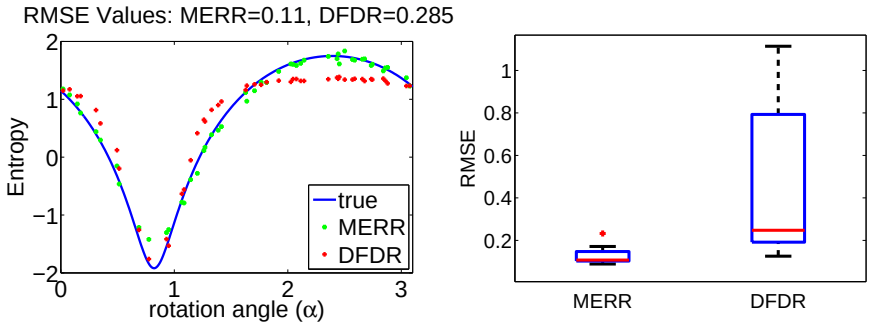
- $\boxed{3} = \boxed{4}$ in Eq. (34):

– (i)-(ii):

$$\frac{1}{l^2\lambda} = \frac{1}{l\lambda^{\frac{1}{b}}} \Leftrightarrow \frac{1}{l} = \lambda^{1-\frac{1}{b}=\frac{b-1}{b}} \Leftrightarrow \frac{1}{l^{\frac{b}{b-1}}} = \lambda \to 0, \text{ if } l \to \infty \quad [\Leftarrow \frac{b}{b-1} > 0].$$

$$r(l,N) = \frac{l^{\frac{3b}{b-1}}\log^h(l)}{N^h} + \frac{1}{l^{\frac{bc}{b-1}}} + \frac{l^{\frac{b}{b-1}}}{l^2} \Rightarrow r(N) = \frac{\log^h(N)}{N^{h-\frac{3ab}{b-1}}} + \frac{1}{N^{\frac{abc}{b-1}}} + \frac{1}{N^{2a-\frac{ab}{b-1}}}.$$

Here,



(a) Entropy of Gaussian (b) Boxplot of RMSE

Figure 1: (a) Learned entropy of a one-dimensional marginal distribution of a rotated 2d Gaussian. Axes x: rotation angle in $[0, \pi]$. Axis y: entropy. (b) RMSE values of the MERR and DFDR algorithms. Boxplots are calculated from 25 experiments.

* (ii): $r(N) \to 0$ if
  - $\boxed{1} \to 0$: Since $h > 0$ we get $h - \frac{3ab}{b-1} > 0$, i.e., $\frac{h(b-1)}{3b} > a$ using that $3b > 0$ and $b - 1 > 0$.
  - $\boxed{2} \to 0$: $\frac{abc}{b-1} > 0$. This requirement holds by our assumptions [$a > 0$, $b > 1$, $c > 0$].
  - $\boxed{3} \to 0$: $2a - \frac{ab}{b-1} > 0$. By $a > 0$ and $b-1 > 0$, this constraint is $2 > \frac{b}{b-1} \Leftrightarrow 2b-2 > b \Leftrightarrow b > 2$.

  Hence, we need $\frac{h(b-1)}{3b} > a$, $b > 2$.
* (i): $N^a \left(\frac{1}{N^{\frac{ab}{b-1}}} \right)^{\frac{b+1}{b}} \geq 1 \Leftrightarrow N^{a - a\frac{b+1}{b-1}} \geq 1$. Thus we need $a - a\frac{b+1}{b-1} > 0 \Leftrightarrow 1 - 1\frac{b+1}{b-1} > 0 \Leftrightarrow 1 > \frac{b+1}{b-1}$, where we used that $a > 0$. The $1 > \frac{b+1}{b-1}$ is never satisfied since $\frac{b+1}{b-1} > 1$.

A.2 Numerical Experiments: Aerosol Prediction

In this section we provide numerical results to demonstrate the efficiency of the analysed ridge regression technique. The experiments serve to illustrate that the MERR approach compares favourably to

1. the only alternative, theoretically justified distribution regression method (since it avoids density estimation);[3] see Section A.2.1,
2. modern domain-specific, engineered methods (which beat state-of-the-art multiple instance learning alternatives); see Section A.2.2.

In our experiments we used the ITE toolbox (Information Theoretical Estimators; [43]).[11]

A.2.1 Supervised entropy learning

We compare our MERR (RKHS based mean embedding ridge regression) algorithm with [1]'s DFDR (kernel smoothing based distribution free distribution regression) method, on a benchmark problem taken from the latter paper. The goal is to learn the entropy of Gaussian distributions in a supervised way. We chose an $A \in \mathbb{R}^{2\times 2}$ matrix, whose A_{ij} entries were uniformly distributed on $[0, 1]$ ($A_{ij} \sim U[0, 1]$). We constructed 100 sample sets from $\{N(0, \Sigma_u)\}_{u=1}^{100}$, where $\Sigma_u = R(\beta_u)AA^T R(\beta_u)^T$ and $R(\beta_u)$ was a 2d rotation matrix with angle $\beta_u \sim U[0, \pi]$. From each $N(0, \Sigma_u)$ distribution we sampled 500 2-dimensional i.i.d. points. From the 100 sample sets, 25 were used for training, 25 for validation (i.e., selecting appropriate parameters), and 50 points for testing. Our goal is to learn the entropy of the first marginal distribution: $H = \frac{1}{2}\ln(2\pi e\sigma^2)$, where $\sigma^2 = M_{1,1}$, $M = \Sigma_u \in \mathbb{R}^{2\times 2}$. Figure 1(a) displays the learned entropies of the 50 test sample sets in a typical experiment. We compare the results of DFDR and MERR. One can see that the true and the estimated values are close to each other for both algorithms, but MERR performs better. The boxplot diagrams of the RMSE (root mean square error)

[11] The ITE toolbox contains the MERR method and its numerical demonstrations (among others); see `https://bitbucket.org/szzoli/ite/`.

Table 4: Prediction accuracy of the MERR method in AOD prediction using different kernels: $100 \times RMSE(\pm std)$. K: linear. The best single and ensemble predictions are written in bold.

k_G	k_e	k_C	k_t	$k_p(p=2)$	$k_p(p=3)$
7.97 ($\pm$1.81)	8.25 ($\pm$1.92)	7.92 ($\pm$1.69)	8.73 ($\pm$2.18)	12.5 ($\pm$2.63)	171.24 ($\pm$56.66)
k_r	k_i	$k_{M,\frac{3}{2}}$	$k_{M,\frac{5}{2}}$	ensemble	
9.66 ($\pm$2.68)	**7.91** ($\pm$**1.61**)	8.05 ($\pm$1.83)	7.98 ($\pm$1.75)	**7.86** ($\pm$**1.71**)	

values calculated from 25 experiments confirm this performance advantage (Figure 1(b)). A reason why MERR achieves better performance is that DFDR needs to do many density estimations, which can be very challenging when the sample sizes are small. By contrast, the MERR algorithm does not require density estimation.

A.2.2 Aerosol prediction

Aerosol prediction is one of the largest challenges of current climate research; we chose this problem as a further testbed of our method. [35] pose the AOD (aerosol optical depth) prediction problem as a MIL task: (i) a given pixel of a multispectral image corresponds to a small area of $200 \times 200m^2$, (ii) spatial variability of AOD can be considered to be small over distances up to $100km$, (iii) ground-based instruments provide AOD labels ($y_i \in \mathbb{R}$), (iv) a bag consists of randomly selected pixels within a $20km$ radius around an AOD sensor. The MIL task can be tackled using our MERR approach, assuming that (i) bags correspond to distributions (x_i), (ii) instances in the bag ($\{x_{i,n}\}_{n=1}^{N}$) are samples from the distribution.

We selected the MISR1 dataset [35], where (i) cloudy pixels are also included, (ii) there are 800 bags with (iii) 100 instances in each bag, (iv) the instances are 16-dimensional ($x_{i,n} \in \mathbb{R}^{16}$). Our baselines are the reported state-of-the-art EM (expectation-maximization) methods achieving average $100 \times RMSE = 7.5 - 8.5$ ($\pm 0.1 - 0.6$) accuracy. The experimental protocol followed the original work, where 5-fold cross-validation (4×160 (160) samples for training (testing)) was repeated 10 times; the only difference is that we made the problem a bit harder, as we used only 3×160 samples for training, 160 for validation (i.e., setting the λ regularization and the θ kernel parameter), and 160 for testing.

- Linear K: In the first set of experiments, K was linear. To study the robustness of our method, we picked 10 different kernels (k) and their ensembles: the Gaussian, exponential, Cauchy, generalized t-student, polynomial kernel of order 2 and 3 ($p = 2$ and 3), rational quadratic, inverse multiquadratic kernel, Matérn kernel (with $\frac{3}{2}$ and $\frac{5}{2}$ smoothness parameters). The expressions for these kernels are

$$k_G(a,b) = e^{-\frac{\|a-b\|_2^2}{2\theta^2}}, \qquad k_e(a,b) = e^{-\frac{\|a-b\|_2}{2\theta^2}}, \qquad k_C(a,b) = \frac{1}{1+\frac{\|a-b\|_2^2}{\theta^2}},$$

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

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

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

  where $p = 2, 3$ and $\theta > 0$. The explored parameter domain was $(\lambda, \theta) \in \{2^{-65}, 2^{-64}, \ldots, 2^{-3}\} \times \{2^{-15}, 2^{-14}, \ldots, 2^{10}\}$; increasing the domain further did not improve the results.

  Our results are summarized in Table 4. According to the table, we achieve $100 \times RMSE = 7.91$ (± 1.61) using a single kernel, or 7.86 (± 1.71) with ensemble of kernels (further performance improvements might be obtained by learning the weights).

- Nonlinear K: We also studied the efficiency of nonlinear K-s. In this case, the argument of K was $\|\mu_a - \mu_b\|_H$ instead of $\|a-b\|_2$ (see the definition of k-s); for K examples, see Table 1. Our obtained

Table 5: Prediction accuracy of the MERR method in AOD prediction using different kernels: $100 \times RMSE(\pm std)$; single prediction case. K: nonlinear. Rows: kernel k. Columns: kernel K. For each row (k), the smallest RMSE value is written in bold.

$k \backslash K$	K_G	K_e	K_C	K_t	$K_{M,\frac{3}{2}}$
k_e	8.14 ($\pm$1.80)	8.10 ($\pm$1.81)	8.14 ($\pm$1.81)	**8.07** (**$\pm$1.77**)	8.09 ($\pm$1.88)
k_C	7.97 ($\pm$1.58)	8.13 ($\pm$1.79)	7.96 ($\pm$1.62)	8.09 ($\pm$1.69)	**7.90** (**$\pm$1.63**)
$k_{M,\frac{3}{2}}$	8.00 ($\pm$1.66)	8.14 ($\pm$1.80)	8.00 ($\pm$1.69)	8.08 ($\pm$1.72)	**7.96** (**$\pm$1.69**)
k_i	8.01 ($\pm$1.53)	8.17 ($\pm$1.74)	8.03 ($\pm$1.63)	7.93 ($\pm$1.57)	8.04 ($\pm$1.67)
$k \backslash K$	$K_{M,\frac{5}{2}}$	K_r	K_i	linear	
k_e	8.14 ($\pm$1.78)	8.12 ($\pm$1.81)	8.12 ($\pm$1.80)	8.25 ($\pm$1.92)	
k_C	7.95 ($\pm$1.60)	7.92 ($\pm$1.61)	7.93 ($\pm$1.61)	7.92 ($\pm$1.69)	
$k_{M,\frac{3}{2}}$	8.02 ($\pm$1.71)	8.04 ($\pm$1.69)	7.98 ($\pm$1.72)	8.05 ($\pm$1.83)	
k_i	8.05 ($\pm$1.61)	8.05 ($\pm$1.63)	8.06 ($\pm$1.65)	**7.91**(**$\pm$1.61**)	

results are summarized in Table 5. One can see that using nonlinear K kernels, the RMSE error drops to 7.90 ($\pm$1.63) in the single prediction case, and decreases further to 7.81 ($\pm$1.64) in the ensemble setting.

Despite the fact that MERR has no domain-specific knowledge wired in, the results fall within the same range as [35]'s algorithms. The prediction is fairly precise and robust to the choice of the kernel, however polynomial kernels perform poorly (they violate our boundedness assumption).