

① Kernel trick:

Def: $k: X \times X \rightarrow \mathbb{R}$ is a reproducing kernel if $\forall n \in \mathbb{N}, \forall x_1, \dots, x_n \in X$, the gram matrix $(G_{ij})_{ij}$ with $G_{ij} = k(x_i, x_j)$ is positive semi-definite.

Thm: [Moore, Aronszajn]
 k reproducing kernel $\Leftrightarrow \exists$ (essentially unique) pair $(\mathcal{H}_k, \gamma_k)$ such that $k(\cdot, \cdot) = \langle \gamma_k(\cdot), \gamma_k(\cdot) \rangle_{\mathcal{H}_k}$.
 ↑ \mathcal{H}_k RKHS ↑ feature map

② Kernels for PDs:

X : space of diagrams
 $k: X \times X \rightarrow \mathbb{R}$ kernel
 γ_k : feature map
 \mathcal{H}_k : RKHS, $\langle \cdot, \cdot \rangle_{\mathcal{H}_k}, \|\cdot\|_{\mathcal{H}_k}$
 $\forall D, D' \in X, \|\gamma_k(D) - \gamma_k(D')\|_{\mathcal{H}_k} \leq C \cdot d_B^{\alpha}(D, D')$ or $C \cdot W_p(D, D')$.

- stability: $\forall D, D' \in X, \|\gamma_k(D) - \gamma_k(D')\|_{\mathcal{H}_k} \leq C \cdot d_B^{\alpha}(D, D')$
- discriminativity: $\forall D, D' \in X, \|\gamma_k(D) - \gamma_k(D')\|_{\mathcal{H}_k} \geq c \cdot d_B^{\alpha}(D, D')$
- injectivity: $\gamma_k: X \rightarrow \mathcal{H}_k$ is injective
- universality: $\mathcal{H}_k := \text{span} \{ k_x: x \in X \}$ is dense in $C^0(X, \mathbb{R})$.
- additivity: $k(D \cup D', D'') = k(D, D'') + k(D', D'') \forall D, D', D'' \in X$.

→ overkill → characteristic: the mean map $\mu \mapsto \mu_{\mathcal{H}_k} = \int_{\text{set } \mathcal{H}_k} [k_x]$ (push-forward measure on X) is injective

reminder:

$d(M: A \leftrightarrow B) = \max \left\{ \sup_{(a,b) \in M} \|a - b\|_{\infty}, \sup_{s \in A \cup B} \|s - \bar{s}\|_{\infty} \right\}$
 → $C_p(M: A \leftrightarrow B) = \left(\sum_{(a,b) \in M} \|a - b\|_{\infty}^p + \sum_{s \in A \cup B} \|s - \bar{s}\|_{\infty}^p \right)^{1/p}$ (other proj. onto \mathcal{H})
 → $W_p(A, B) = \inf_{M: A \leftrightarrow B} C_p(M)$

③ Landscapes:

Note: pts at infinity are removed.

$$D \mapsto \Delta_D : \mathbb{N} \times \mathbb{R} \rightarrow \mathbb{R}$$

$$\Delta_D \in L^2(\mathbb{N} \times \mathbb{R})$$

\hookrightarrow equipped with the product of $\begin{matrix} \mu \\ \nu \end{matrix}$ $\begin{matrix} \rightarrow \text{counting measure on } \mathbb{N} \\ \rightarrow \text{Lebesgue measure on } \mathbb{R} \end{matrix}$

$$\int_{\mathbb{N} \times \mathbb{R}} \Delta_D d\mu := \sum_{k=1}^{\infty} \int_{\mathbb{R}} \Delta_D(k, t) dt$$

Note: $\sum_k \int_{\mathbb{R}} \Delta_D(k, t)^2 dt < +\infty$ ~~iff~~ when $|D|$ is finite.

ie: $\Delta_D \in L^2(\mathbb{N} \times \mathbb{R})$ when $|D|$ is finite.

④ Discrete measures:

$$D = \sum_{p \in D} \delta_p \quad (\text{no renormalization})$$

Heat equation: ~~with~~ $u : \mathbb{R}^2 \times \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$

$$\left\{ \begin{array}{l} \frac{\partial u(x, t)}{\partial t} = \Delta_x u(x, t) \end{array} \right.$$

$u|_{x \in \partial} = 0 \quad \forall x \in \Delta \text{ (diagonal) and } t \in \mathbb{R}_{\geq 0} \text{ (Dirichlet cond.)}$

$$u|_{t=0} = \sum_{p \in D} \delta_p - \delta_{\bar{p}}$$

$\hookrightarrow \phi_k := \text{solution } u|_{t=0}$

$\hookrightarrow k := \langle \phi_k(\cdot), \phi_k(\cdot) \rangle_{L^2(\mathbb{R}^2)}$

⑤ Bootstrap:

- View \hat{X}_n itself as an observation of a random variable $\sim \mu^{\otimes n}$ (n pts sampled iid according to μ)
- Study the statistics of $d_B(D_g \hat{F}(\hat{X}_n), D_g \hat{F}(X))$.
measures the amplitude of variation of $D_g \hat{F}(\hat{X}_n)$ around $D_g \hat{F}(X)$ in the space of diagrams.

• Main idea:

The above statistics is similar to the one of

$$d_B(D_g \hat{F}(\hat{X}^*), D_g \hat{F}(\hat{X}_n))$$

\uparrow
 $\mu_{\hat{X}_n}^{\otimes n}$
 \uparrow
empirical measure on \hat{X}_n

(n pts drawn from \hat{X}_n with unif. proba. and with replacement)

• $(1-\epsilon)$ quantile:

$$\hat{q}_\epsilon := \inf \left\{ t : \frac{1}{N} \sum_{i=1}^N \mathbb{I}(\sqrt{n} d_i^* \geq t) \leq \epsilon \right\}$$

$$= \begin{cases} 1 & \text{if } \sqrt{n} d_i^* \geq t \\ 0 & \text{otherwise} \end{cases}$$