

Two-stage Sampled Learning Theory on Distributions

Zoltán Szabó (Gatsby Unit, UCL)

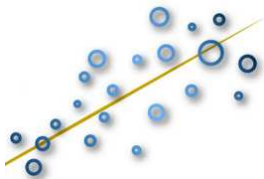
Joint work with

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The task

- Samples: $\{(x_i, y_i)\}_{i=1}^{\ell}$. Wanted: $f \in \mathcal{H}$ such that $f(x_i) \approx y_i$.



- Distribution regression:
 - x_i -s are distributions,
 - available only through samples: $\{x_{i,n}\}_{n=1}^{N_i}$.
- \Rightarrow Training examples: labelled *bags*.

Example: aerosol prediction from satellite images

- Bag := pixels of a multispectral satellite image over an area.
- Label of a bag := aerosol value.



- Relevance: climate research.
- Engineered methods [Wang et al., 2012]: $100 \times \text{RMSE} = 7.5 - 8.5$.
- Using distribution regression?

- Context:
 - machine learning: multi-instance learning,
 - statistics: point estimation tasks (without analytical formula).



- Applications:
 - computer vision: image = collection of patch **vectors**,
 - network analysis: group of people = bag of friendship **graphs**,
 - natural language processing: corpus = bag of **documents**,
 - time-series modelling: user = set of trial **time-series**.

Several algorithmic approaches

- 1 Parametric fit: Gaussian, MOG, exp. family
[Jebara et al., 2004, Wang et al., 2009, Nielsen and Nock, 2012].
- 2 Kernelized Gaussian measures:
[Jebara et al., 2004, Zhou and Chellappa, 2006].
- 3 (Positive definite) kernels:
[Cuturi et al., 2005, Martins et al., 2009, Hein and Bousquet, 2005].
- 4 Divergence measures (KL, Rényi, Tsallis): [Póczos et al., 2011].
- 5 Set metrics: Hausdorff metric [Edgar, 1995]; variants
[Wang and Zucker, 2000, Wu et al., 2010, Zhang and Zhou, 2009, Chen and Wu, 2012].

Theoretical guarantee?

- MIL dates back to [Haussler, 1999, Gärtner et al., 2002].



- *Sensible* methods in regression: require density estimation [Póczos et al., 2013, Oliva et al., 2014, Reddi and Póczos, 2014]
+ assumptions:
 - 1 compact Euclidean domain.
 - 2 output = \mathbb{R} ([Oliva et al., 2013] allows distribution).

- $k : \mathcal{D} \times \mathcal{D} \rightarrow \mathbb{R}$ kernel on \mathcal{D} , if
 - $\exists \varphi : \mathcal{D} \rightarrow H$ (ilbert space) feature map,
 - $k(a, b) = \langle \varphi(a), \varphi(b) \rangle_H$ ($\forall a, b \in \mathcal{D}$).

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- Kernel examples: $\mathcal{D} = \mathbb{R}^d$ ($p > 0, \theta > 0$)
 - $k(a, b) = (\langle a, b \rangle + \theta)^p$: polynomial,
 - $k(a, b) = e^{-\|a-b\|_2^2 / (2\theta^2)}$: Gaussian,
 - $k(a, b) = e^{-\theta \|a-b\|_1}$: Laplacian.
- In the $H = H(k)$ RKHS ($\exists!$): $\varphi(u) = k(\cdot, u)$.

Kernel: example domains (\mathcal{D})

- Euclidean space: $\mathcal{D} = \mathbb{R}^d$.
- Graphs, texts, time series, dynamical systems.



- **Distributions!**

Problem formulation

- Given:

- labelled bags $\hat{\mathbf{z}} = \{(\hat{x}_i, y_i)\}_{i=1}^{\ell}$,

- i^{th} bag: $\hat{x}_i = \{x_{i,1}, \dots, x_{i,N}\} \stackrel{i.i.d.}{\sim} x_i \in \mathcal{P}(\mathcal{D}), y_i \in \mathbb{R}$.

- Task: find a $\mathcal{P}(\mathcal{D}) \rightarrow \mathbb{R}$ mapping based on $\hat{\mathbf{z}}$.

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$$\mathcal{P}(\mathcal{D}) \xrightarrow{\mu = \mu(k)} X \subseteq H = H(k)$$

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- Our goal: risk bound compared to the regression function

$$f_{\rho}(\mu_x) = \int_{\mathbb{R}} y d\rho(y|\mu_x).$$

- Expected risk:

$$\mathcal{R}[f] = \mathbb{E}_{(x,y)} |f(\mu_x) - y|^2.$$

- Contribution: analysis of the excess risk

$$\mathcal{E}(f_{\hat{\mathbf{z}}}^\lambda, f_\rho) = \mathcal{R}[f_{\hat{\mathbf{z}}}^\lambda] - \mathcal{R}[f_\rho]$$

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$$f_{\hat{z}}^\lambda = \arg \min_{f \in \mathcal{H}} \frac{1}{\ell} \sum_{i=1}^{\ell} |f(\mu_{\hat{x}_i}) - y_i|^2 + \lambda \|f\|_{\mathcal{H}}^2, \quad (\lambda > 0).$$

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- We consider the well-specified assumption: $f_{\rho} \in \mathcal{H}$.

Step-1: mean embedding

- $k : \mathcal{D} \times \mathcal{D} \rightarrow \mathbb{R}$ kernel; canonical feature map: $\varphi(u) = k(\cdot, u)$.
- Mean embedding of a distribution $x, \hat{x}_i \in \mathcal{P}(\mathcal{D})$:

$$\mu_x = \int_{\mathcal{D}} k(\cdot, u) dx(u) \in H(k),$$
$$\mu_{\hat{x}_i} = \frac{1}{N} \sum_{n=1}^N k(\cdot, x_{i,n}).$$

- Linear $K \Rightarrow$ set kernel:

$$K(\mu_{\hat{x}_i}, \mu_{\hat{x}_j}) = \langle \mu_{\hat{x}_i}, \mu_{\hat{x}_j} \rangle_H = \frac{1}{N^2} \sum_{n,m=1}^N k(x_{i,n}, x_{j,m}).$$

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- Nonlinear K example:

$$K(\mu_{\hat{x}_i}, \mu_{\hat{x}_j}) = e^{-\frac{\|\mu_{\hat{x}_i} - \mu_{\hat{x}_j}\|_H^2}{2\sigma^2}}.$$

Step-2: ridge regression (analytical solution)

- Given:
 - training sample: $\hat{\mathbf{z}}$,
 - test distribution: t .
- Prediction on t :

$$(f_{\hat{\mathbf{z}}}^\lambda \circ \mu)(t) = \mathbf{k}(\mathbf{K} + \ell\lambda\mathbf{I}_\ell)^{-1}[y_1; \dots; y_\ell], \quad (1)$$

$$\mathbf{K} = [K(\mu_{\hat{x}_i}, \mu_{\hat{x}_j})] \in \mathbb{R}^{\ell \times \ell}, \quad (2)$$

$$\mathbf{k} = [K(\mu_{\hat{x}_1}, \mu_t), \dots, K(\mu_{\hat{x}_\ell}, \mu_t)] \in \mathbb{R}^{1 \times \ell}. \quad (3)$$

Blanket assumptions

- \mathcal{D} : separable, topological domain.
- k :
 - bounded: $\sup_{u \in \mathcal{D}} k(u, u) \leq B_k \in (0, \infty)$,
 - continuous.
- K : bounded; Hölder continuous: $\exists L > 0, h \in (0, 1]$ such that

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

- y : bounded.
- $X = \mu(\mathcal{P}(\mathcal{D})) \in \mathcal{B}(H)$.

Performance guarantee (in human-readable format)

- Difficulty of the task:
 - f_ρ is 'c-smooth',
 - ' b -decaying covariance operator'.
- Contribution: If $\ell \geq \lambda^{-\frac{1}{b}-1}$, then with high probability

$$\mathcal{E}(f_{\frac{1}{2}}^\lambda, f_\rho) \leq \underbrace{\frac{\log^h(\ell)}{N^h \lambda^3} + \lambda^c + \frac{1}{\ell^2 \lambda} + \frac{1}{\ell \lambda^{\frac{1}{b}}}}_{g(\ell, N, \lambda)}.$$

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The diagram illustrates the components of the performance guarantee. A box labeled \hat{x}_i points to the fraction $\frac{\log^h(\ell)}{N^h \lambda^3}$. A box labeled c -smoothness points to the λ^c term. A bracket under the terms $\lambda^c + \frac{1}{\ell^2 \lambda} + \frac{1}{\ell \lambda^{\frac{1}{b}}}$ is labeled $g(\ell, N, \lambda)$.

Performance guarantee: example

Assume

- b is 'large' ($1/b \approx 0$, 'small' effective input dimension),
- $h = 1$ (K : Lipschitz),
- $\boxed{1} = \boxed{2}$ in (4) $\Rightarrow \lambda; \ell = N^a$ ($a > 0$),
- $t = \ell N$: total number of samples processed.

Then

- 1 $c = 2$ ('smooth' f_ρ): $\mathcal{E}(f_{\frac{1}{2}}^\lambda, f_\rho) \approx t^{-\frac{2}{7}}$ – faster convergence,
- 2 $c = 1$ ('non-smooth' f_ρ): $\mathcal{E}(f_{\frac{1}{2}}^\lambda, f_\rho) \approx t^{-\frac{1}{5}}$ – slower.

Hölder K examples

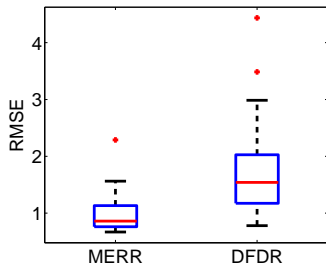
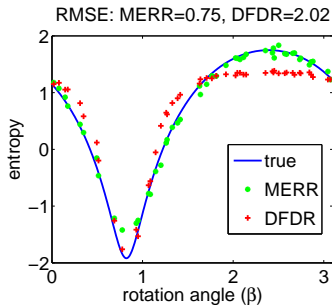
In case of compact metric \mathcal{D} , universal k :

K_G	K_e	K_C
$e^{-\frac{\ \mu_a - \mu_b\ _H^2}{2\theta^2}}$	$e^{-\frac{\ \mu_a - \mu_b\ _H}{2\theta^2}}$	$\left(1 + \ \mu_a - \mu_b\ _H^2 / \theta^2\right)^{-1}$
$h = 1$	$h = \frac{1}{2}$	$h = 1$

K_t	K_i
$\left(1 + \ \mu_a - \mu_b\ _H^\theta\right)^{-1}$	$\left(\ \mu_a - \mu_b\ _H^2 + \theta^2\right)^{-\frac{1}{2}}$
$h = \frac{\theta}{2} \ (\theta \leq 2)$	$h = 1$

They are functions of $\|\mu_a - \mu_b\|_H \Rightarrow$ computation: similar to set kernel.

- Supervised entropy learning:



- Aerosol prediction from satellite images:
 - State-of-the-art baseline: **7.5 – 8.5** ($\pm 0.1 – 0.6$).
 - MERR: **7.81** (± 1.64).

- Problem: distribution regression.
- Literature: large number of heuristics.
- Contribution:
 - a simple ridge solution is consistent,
 - specifically, the set kernel is so (15-year-old open question).
- Code in ITE, extended analysis (submitted to JMLR):

<https://bitbucket.org/szzoli/ite/>

<http://arxiv.org/abs/1411.2066>.

Thank you for the attention!



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- Topological definitions, separability.
- Prior definition (ρ).
- $\exists \rho, X \in \mathcal{B}(H)$.
- Universal kernel examples.
- Demos: further details.
- Hausdorff metric.
- Weak topology on $\mathcal{P}(\mathcal{D})$.

- Given: $\mathcal{D} \neq \emptyset$ set.
- $\tau \subseteq 2^{\mathcal{D}}$ is called a *topology* on \mathcal{D} if:
 - 1 $\emptyset \in \tau, \mathcal{D} \in \tau$.
 - 2 Finite intersection: $O_1 \in \tau, O_2 \in \tau \Rightarrow O_1 \cap O_2 \in \tau$.
 - 3 Arbitrary union: $O_i \in \tau (i \in I) \Rightarrow \cup_{i \in I} O_i \in \tau$.

Then, (\mathcal{D}, τ) is called a *topological space*; $O \in \tau$: *open sets*.

Given: (\mathcal{D}, τ) . $A \subseteq \mathcal{D}$ is

- *closed* if $\mathcal{D} \setminus A \in \tau$ (i.e., its complement is open),
- *compact* if for any family $(O_i)_{i \in I}$ of open sets with $A \subseteq \bigcup_{i \in I} O_i$, $\exists i_1, \dots, i_n \in I$ with $A \subseteq \bigcup_{j=1}^n O_{i_j}$.

Closure of $A \subseteq \mathcal{D}$:

$$\bar{A} := \bigcap_{A \subseteq C \text{ closed in } \mathcal{D}} C. \quad (4)$$

- $A \subseteq \mathcal{D}$ is *dense* if $\bar{A} = \mathcal{D}$.
- (\mathcal{D}, τ) is *separable* if \exists countable, dense subset of \mathcal{D} .
Counterexample: l^∞ / L^∞ .

- Let the $T : \mathcal{H} \rightarrow \mathcal{H}$ covariance operator be

$$T = \int_{\mathcal{X}} K(\cdot, \mu_a) K^*(\cdot, \mu_a) d\rho_X(\mu_a)$$

with eigenvalues t_n ($n = 1, 2, \dots$).

- Assumption: $\rho \in \mathcal{P}(b, c)$ = set of distributions on $X \times Y$
 - $\alpha \leq n^b t_n \leq \beta$ ($\forall n \geq 1; \alpha > 0, \beta > 0$),
 - $\exists g \in \mathcal{H}$ such that $f_\rho = T^{\frac{c-1}{2}} g$ with $\|g\|_{\mathcal{H}}^2 \leq R$ ($R > 0$),where $b \in (1, \infty)$, $c \in [1, 2]$.

- Intuition: $1/b$ – effective input dimension, c – smoothness of f_ρ .

Notes on the assumptions: $\exists \rho, X \in \mathcal{B}(H)$

- k : bounded, continuous \Rightarrow
 - $\mu : (\mathcal{P}(\mathcal{D}), \mathcal{B}(\tau_w)) \rightarrow (H, \mathcal{B}(H))$ measurable.
 - μ measurable, $X \in \mathcal{B}(H) \Rightarrow \rho$ on $X \times Y$: well-defined.
- If $(*) := \mathcal{D}$ is compact metric, k is universal, then
 - μ is continuous, and
 - $X \in \mathcal{B}(H)$.

- Def.: $k : \mathcal{D} \times \mathcal{D} \rightarrow \mathbb{R}$ kernel is universal if
 - it is continuous,
 - $H(k)$ is dense in $(C(\mathcal{D}), \|\cdot\|_\infty)$.
- Examples: on compact subsets of \mathbb{R}^d

$$k(a, b) = e^{-\frac{\|a-b\|_2^2}{2\sigma^2}}, \quad (\sigma > 0)$$

$$k(a, b) = e^{-\sigma\|a-b\|_1}, \quad (\sigma > 0)$$

$$k(a, b) = e^{\beta\langle a, b \rangle}, \quad (\beta > 0), \text{ or more generally}$$

$$k(a, b) = f(\langle a, b \rangle), \quad f(x) = \sum_{n=0}^{\infty} a_n x^n \quad (\forall a_n > 0)$$

Demo-1: supervised entropy learning

- Problem: learn the entropy of the 1st coo. of (rotated) Gaussians.
- Baseline: kernel smoothing based distribution regression (applying density estimation) =: DFDR.
- Performance: RMSE boxplot over 25 random experiments.
- Experience:
 - more precise than the only theoretically justified method,
 - by avoiding density estimation.

Demo-2: aerosol prediction – picked kernels

Kernel definitions ($p = 2, 3$):

$$k_G(a, b) = e^{-\frac{\|a-b\|_2^2}{2\theta^2}}, \quad k_e(a, b) = e^{-\frac{\|a-b\|_2}{2\theta^2}}, \quad (5)$$

$$k_C(a, b) = \frac{1}{1 + \frac{\|a-b\|_2^2}{\theta^2}}, \quad k_t(a, b) = \frac{1}{1 + \|a-b\|_2^\theta}, \quad (6)$$

$$k_p(a, b) = (\langle a, b \rangle + \theta)^p, \quad k_r(a, b) = 1 - \frac{\|a-b\|_2^2}{\|a-b\|_2^2 + \theta}, \quad (7)$$

$$k_i(a, b) = \frac{1}{\sqrt{\|a-b\|_2^2 + \theta^2}}, \quad (8)$$

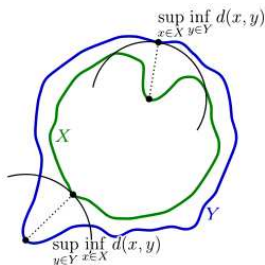
$$k_{M, \frac{3}{2}}(a, b) = \left(1 + \frac{\sqrt{3} \|a-b\|_2}{\theta}\right) e^{-\frac{\sqrt{3} \|a-b\|_2}{\theta}}, \quad (9)$$

$$k_{M, \frac{5}{2}}(a, b) = \left(1 + \frac{\sqrt{5} \|a-b\|_2}{\theta} + \frac{5 \|a-b\|_2^2}{3\theta^2}\right) e^{-\frac{\sqrt{5} \|a-b\|_2}{\theta}}. \quad (10)$$

Existing methods: set metric based algorithms

- Hausdorff metric [Edgar, 1995]:

$$d_H(X, Y) = \max \left\{ \sup_{x \in X} \inf_{y \in Y} d(x, y), \sup_{y \in Y} \inf_{x \in X} d(x, y) \right\}. \quad (11)$$




- Metric on compact sets of metric spaces $[(M, d); X, Y \subseteq M]$.
- 'Slight' problem: highly sensitive to outliers.

Def.: It is the weakest topology such that the


$$L_h : (\mathcal{P}(\mathcal{D}), \tau_w) \rightarrow \mathbb{R},$$
$$L_h(x) = \int_{\mathcal{D}} h(u) dx(u)$$


mapping is continuous for all $h \in C_b(\mathcal{D})$, where


$$C_b(\mathcal{D}) = \{(\mathcal{D}, \tau) \rightarrow \mathbb{R} \text{ bounded, continuous functions}\}.$$





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