# Consistent Vector-valued Regression on Probability Measures

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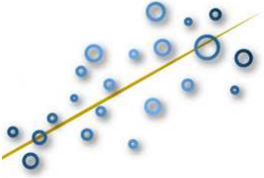
# The task

- Samples: $\{(x_i, y_i)\}_{i=1}^{l}$. Goal: $f(x_i) \approx y_i$, find $f \in \mathcal{H}$.



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

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

# Wider context

- 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] + assumptions:
    1. compact Euclidean domain.
    2. output = $\mathbb{R}$.

# Problem formulation

- Given: labelled bags
  - $\hat{\mathbf{z}} = \{(\hat{x}_i, y_i)\}_{i=1}^{l}$, where
  - $i^{th}$ bag: $\hat{x}_i = \{x_{i,1}, \ldots, x_{i,N}\} \overset{i.i.d.}{\sim} x_i \in \mathcal{M}_1^+(\mathcal{D})$, $y_i \in Y$.
- Task: find a $\mathcal{M}_1^+(\mathcal{D}) \to Y$ mapping based on $\hat{\mathbf{z}}$.
- Construction: distribution embedding $(\mu_x)$ + ridge regression

$$\mathcal{M}_1^+(\mathcal{D}) \xrightarrow{\mu=\mu(k)} X \subseteq H = H(k) \xrightarrow{f\in\mathcal{H}=\mathcal{H}(K)} Y.$$

- Our goal: risk bound compared to the regression function

$$f_\rho(\mu_x) = \int_Y y \mathrm{d}\rho(y|\mu_x).$$

# Goal in details

Contribution: analysis of the excess risk

$$\mathcal{E}(f_{\hat{\mathbf{z}}}^{\lambda}, f_{\rho}) = \mathcal{R}[f_{\hat{\mathbf{z}}}^{\lambda}] - \mathcal{R}[f_{\rho}] \leq g(l, N, \lambda) \rightarrow 0 \text{ and rates,}$$

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

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

We consider two settings:

1. well-specified case: $f_{\rho} \in \mathcal{H}$,
2. misspecified case: $f_{\rho} \in L_{\rho_X}^2 \backslash \mathcal{H}$.

# Kernel, step-1 = mean embedding

- $k : \mathcal{D} \times \mathcal{D} \to \mathbb{R}$ kernel; canonical feature map: $\varphi(u) = k(\cdot, u)$.
- Mean embedding of a distribution $x, \hat{x}_i \in \mathcal{M}_1^+(\mathcal{D})$:

$$\mu_x = \int_{\mathcal{D}} k(\cdot, u) \mathrm{d}x(u) \in H(k),$$

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

- $Y = \mathbb{R}$, linear $K \Rightarrow$ set kernel:

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

# Vector-valued RKHS: $\mathcal{H} = \mathcal{H}(K)$

Definition:

- A $\mathcal{H} \subseteq Y^X$ Hilbert space of functions is RKHS if

$$A_{\mu_x,y} : f \in \mathcal{H} \mapsto \langle y, f(\mu_x) \rangle_Y \in \mathbb{R} \tag{1}$$

  is *continuous* for $\forall \mu_x \in X, y \in Y$.

- $=$ The evaluation functional is continuous in every direction.

# Vector-valued RKHS: $\mathcal{H} = \mathcal{H}(K)$ – continued

- Riesz representation theorem $\Rightarrow \exists K(\mu_x|y) \in \mathcal{H}$:

$$\langle y, f(\mu_x)\rangle_Y = \langle K(\mu_x|y), f\rangle_{\mathcal{H}} \quad (\forall f \in \mathcal{H}). \tag{2}$$

- $K(\mu_x|y)$: linear, bounded in $y \Rightarrow K(\mu_x|y) = K_{\mu_x}(y)$ with $K_{\mu_x} \in \mathcal{L}(Y, \mathcal{H})$.

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- $K$ construction:

$$K(\mu_x, \mu_t)(y) = (K_{\mu_t} y)(\mu_x), \quad (\forall \mu_x, \mu_t \in X), \text{ i.e.,}$$

$$K(\cdot, \mu_t)(y) = K_{\mu_t} y, \tag{3}$$

$$\mathcal{H}(K) = \overline{span}\{K_{\mu_t} y : \mu_t \in X, y \in Y\}. \tag{4}$$

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- Shortly: $K(\mu_x, \mu_t) \in \mathcal{L}(Y)$ generalizes $k(u, v) \in \mathbb{R}$.

# Vector-valued RKHS – examples: $Y = \mathbb{R}^d$

1. $K_i : X \times X \to \mathbb{R}$ kernels ($i = 1, \ldots, d$). Diagonal kernel:

$$K(\mu_a, \mu_b) = diag(K_1(\mu_a, \mu_b), \ldots, K_d(\mu_a, \mu_b)). \quad (5)$$

2. Combination of $D_j$ diagonal kernels [$D_j(\mu_a, \mu_b) \in \mathbb{R}^{r \times r}$, $A_j \in \mathbb{R}^{r \times d}$]:

$$K(\mu_a, \mu_b) = \sum_{j=1}^{m} A_j^* D_j(\mu_a, \mu_b) A_j. \quad (6)$$

# Step-2 (ridge regression): analytical solution

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

$$(f_{\hat{\mathbf{z}}}^{\lambda} \circ \mu)(t) = \mathbf{k}(\mathbf{K} + l\lambda \mathbf{I}_l)^{-1}[y_1; \ldots; y_l], \tag{7}$$

$$\mathbf{K} = [K(\mu_{\hat{x}_i}, \mu_{\hat{x}_j})] \in \mathcal{L}(Y)^{l \times l}, \tag{8}$$

$$\mathbf{k} = [K(\mu_{\hat{x}_1}, \mu_t), \ldots, K(\mu_{\hat{x}_l}, \mu_t)] \in \mathcal{L}(Y)^{1 \times l}. \tag{9}$$

- Specially: $Y = \mathbb{R} \Rightarrow \mathcal{L}(Y) = \mathbb{R}$; $Y = \mathbb{R}^d \Rightarrow \mathcal{L}(Y) = \mathbb{R}^{d \times d}$.

# Blanket assumptions

- $\mathcal{D}$: separable, topological domain.
- $k$: bounded, continuous.
- $K$: bounded, Hölder continuous.
- $Y$: separable Hilbert.
- $y$: bounded.
- $X = \mu\left(\mathcal{M}_1^+(\mathcal{D})\right) \in \mathcal{B}(H)$.

# Performance guarantees (in human-readable format)

If in addition

1. well-specified case: $f_\rho$ is '$c$-smooth' with '$b$-decaying covariance operator' and $l \geq \lambda^{-\frac{1}{b}-1}$, then

$$\mathcal{E}(f_{\hat{\mathbf{z}}}^{\lambda}, f_\rho) \leq \frac{\log^h(l)}{N^h \lambda^3} + \lambda^c + \frac{1}{l^2 \lambda} + \frac{1}{l \lambda^{\frac{1}{b}}}. \tag{10}$$

2. misspecified case: $f_\rho$ is '$s$-smooth', $L^2_{\rho_X}$ is separable, and $\frac{1}{\lambda^2} \leq l$, then

$$\mathcal{E}(f_{\hat{\mathbf{z}}}^{\lambda}, f_\rho) \leq \frac{\log^{\frac{h}{2}}(l)}{N^{\frac{h}{2}} \lambda^{\frac{3}{2}}} + \frac{1}{\sqrt{l\lambda}} + \frac{\sqrt{\lambda^{\min(1,s)}}}{\lambda \sqrt{l}} + \lambda^{\min(1,s)}. \tag{11}$$

# Performance guarantee: example

Misspecified case: assume

- $s \geq 1$, $h = 1$ ($K$: Lipschitz),
- $\boxed{1} = \boxed{3}$ in (11) $\Rightarrow \lambda$; $l = N^a$ $(a > 0)$
- $t = lN^a$: total number of samples processed.

Then

1. $s = 1$ ('most difficult' task): $\mathcal{E}(f_{\hat{\mathbf{z}}}^{\lambda}, f_{\rho}) \approx t^{-0.25}$,
2. $s \to \infty$ ('simplest' problem): $\mathcal{E}(f_{\hat{\mathbf{z}}}^{\lambda}, f_{\rho}) \approx t^{-0.5}$.

# Notes on the assumptions: $K$

$K$ is

1. bounded:

$$\|K_{\mu_a}\|_{\mathrm{HS}}^2 = Tr\left(K_{\mu_a}^* K_{\mu_a}\right) \le B_K \in (0,\infty), \quad (\forall \mu_a \in X).$$

2. Hölder continuous: $\exists L > 0$, $h \in (0,1]$ such that

$$\|K_{\mu_a} - K_{\mu_b}\|_{\mathcal{L}(Y,\mathcal{H})} \le L \|\mu_a - \mu_b\|_H^h, \quad \forall (\mu_a, \mu_b) \in X \times X.$$

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

- $k$: bounded, continuous $\Rightarrow$
  - $\mu : (\mathcal{M}_1^+(\mathcal{D}), \mathcal{B}(\tau_w)) \to (H, \mathcal{B}(H))$ measurable.
  - $\mu$ measurable, $X \in \mathcal{B}(H) \Rightarrow \rho$ on $X \times Y$: well-defined.
- If (*) := $\mathcal{D}$ is compact metric, $k$ is universal, then $\mu$ is continuous and $X \in \mathcal{B}(H)$.
- If $Y = \mathbb{R}$, we get the traditional boundedness of $K$:

$$K(\mu_a, \mu_a) \leq B_K, \quad (\forall \mu_a \in X).$$

# Notes on the assumptions: $K$ – continued

If (*) and $Y = \mathbb{R}$, then $K$ Hölder kernel examples:

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

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

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

# Notes on the assumptions: $\rho \in \mathcal{P}(b, c)$

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

$$T = \int_X K(\cdot, \mu_a) K^*(\cdot, \mu_a) \mathrm{d}\rho_X(\mu_a)$$

  with eigenvalues $t_n$ $(n = 1, 2, \ldots)$.
- Assumption: $\rho \in \mathcal{P}(b, c)$ = set of distributions on $X \times Y$
  - $\alpha \leq n^b t_n \leq \beta \quad (\forall n \geq 1; \alpha > 0, \beta > 0)$,
  - $\exists g \in \mathcal{H}$ 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: $b$ – effective input dimension, $c$ – smoothness of $f_\rho$.

# Notes on the assumptions: misspecified case

Let $\tilde{T}$ be the extension of $T$ from $\mathcal{H}$ to $L^2_{\rho_X}$:

$$S_K^* : \mathcal{H} \hookrightarrow L^2_{\rho_X},$$

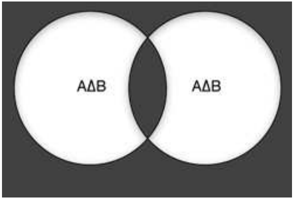
$$S_K : L^2_{\rho_X} \to \mathcal{H}, \quad (S_K g)(\mu_u) = \int_X K(\mu_u, \mu_t) g(\mu_t) \mathrm{d}\rho_X(\mu_t),$$

$$\tilde{T} = S_K^* S_K : L^2_{\rho_X} \to L^2_{\rho_X}.$$

Our range space assumption on $\rho$: $f_\rho \in Im\left(\tilde{T}^s\right)$ for some $s \geq 0$.

# Notes on the assumptions: misspecified case

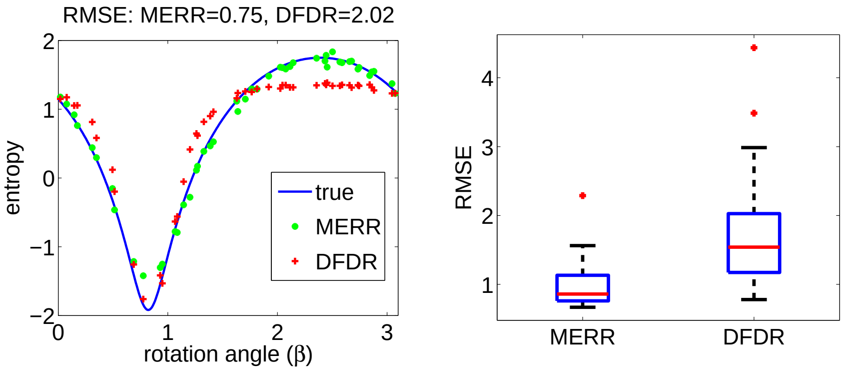
$L^2_{\rho_X}$: separable $\Leftrightarrow$ measure space with $d(A,B) = \rho_X(A \triangle B)$ is so [Thomson et al., 2008].



# Demo-1 ($Y = \mathbb{R}$): Supervised entropy learning

- Problem: learn the entropy 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.

# Supervised entropy learning: plots



# Demo-2 ($Y = \mathbb{R}$): Aerosol prediction from satellite images

- Performance: $100 \times$ RMSE.
- Baseline [mixture model (EM)]: $7.5 - 8.5$ ($\pm 0.1 - 0.6$).
- Linear $K$:
  - single: 7.91 ($\pm$1.61).
  - ensemble: **7.86** ($\pm$**1.71**).
- Nonlinear $K$:
  - Single: 7.90 ($\pm$1.63),
  - Ensemble: **7.81** ($\pm$**1.64**).

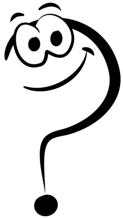
# Summary

- Problem: distribution regression.
- Literature: large number of heuristics.
- Contribution:
  - a simple ridge solution is consistent,
  - specially, the set kernel is so (15-year-old open question).
- Code $\in$ ITE toolbox:

  `https://bitbucket.org/szzoli/ite/`
- Details (submitted to JMLR):

  `http://arxiv.org/pdf/1411.2066`.

Thank you for the attention!



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# Appendix: contents

- Topological definitions, separability.
- Hausdorff metric.
- Weak topology on $\mathcal{M}_1^+(\mathcal{D})$.
- Universal kernel examples.

# Topological space, open sets

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

# Closed-, compact set, closure, dense subset, separability

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

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

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

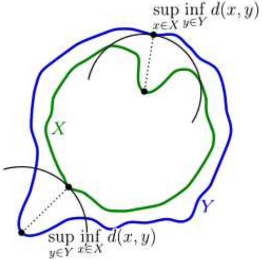
$$\bar{A} := \bigcap_{A \subseteq C \text{ closed in } \mathcal{D}} C. \tag{12}$$

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

# Existing methods: set metric based algorithms

- Hausdorff metric [Edgar, 1995]:

$$d_H(X,Y) = \max\left\{ \sup_{x\in X} \inf_{y\in Y} d(x,y), \sup_{y\in Y} \inf_{x\in X} d(x,y) \right\}. \quad (13)$$




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

# Weak topology on $\mathcal{M}_1^+(\mathcal{D})$

Def.: It is the weakest topology such that the

$$L_h : (\mathcal{M}_1^+(\mathcal{D}), \tau_w) \to \mathbb{R},$$
$$L_h(x) = \int_{\mathcal{D}} h(u) \mathrm{d}x(u)$$

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

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

# Universal kernel examples

On every compact subset of $\mathbb{R}^d$:

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

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

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

$$k(a,b) = (1 - \langle a,b\rangle)^{\alpha}, \quad (\alpha > 0).$$

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