Consistent Distribution Regression via Mean Embedding

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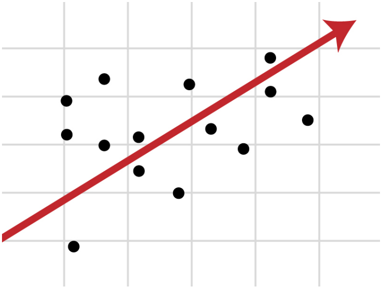
Outline

- Motivation.
- Problem formulation.
- Algorithm, consistency result.
- Numerical illustration.

Regression

- Given: $\{(x_i, y_i)\}_{i=1}^{l}$ samples $\mathcal{H} \ni f =?$ such that $f(x_i) \approx y_i$.



- Typically: $x_i \in \mathbb{R}^p$, $y_i \in \mathbb{R}^q$.
- Our interest: x_i-s are distributions (∞-dimensional objects).

Distribution regression: two-stage sampling difficulty

In practise:

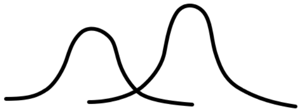
- x_i-s are only observable via samples: $x_i \approx \{x_{i,n}\}_{n=1}^{N} \Rightarrow$
- an x_i is represented as a *bag*:
  - image $=$ set of patches,
  - document $=$ bag of words,
  - video $=$ collection of images,
  - different configurations of a molecule $=$ bag of shapes.

Example: supervised entropy learning

- Entropy of $x \sim f$: $-\int f(u) \log[f(u)] \mathrm{d}u$.
- Training: samples from distributions, entropy values.
- Task: estimate the entropy of a new sample set.

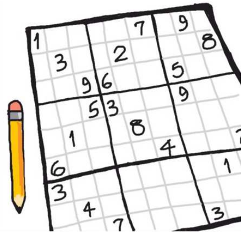
Example: hyperparameter selection

- Training: samples from MOGs with component number labels.
- Task:
  - given: samples from a new MOG distribution,
  - predict: the number of components.



Example: Sudoku difficulty estimation

- Sudoku: special constraint satisfaction problem.
- Spiking neural networks (SNN)
  - can be used to solve such problems,
  - have stationary distribution under mild conditions.
- Sudoku $\leftrightarrow$ stationary distribution of the SNN.

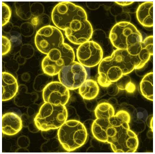


Example: age prediction from images

- Training: (image, age) pairs; image = bag of features.
- Goal: estimate the age of a person being on a new image.

Example: toxic level estimation from tissues

- Toxin alters the properties/causes mutations in cells.
- Training data:
  - bag = tissue,
  - samples in the bag = cells described by some simple features,
  - output label = toxic level.
- Task: predict the toxic level given a new tissue.



Example: aerosol prediction using satellite images

- Aerosol = floating particles in the air; climate research.
- Multispectral satellite images: 1 pixel $= 200 \times 200m^2 \in$ bag.
- Bag label: ground-based (expensive) sensor.
- Task: satellite image $\rightarrow$ aerosol density.

Towards problem formulation: kernel

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

Kernel $\Leftrightarrow$ reproducing kernel Hilbert space (RKHS)

- $k \to H$: not necessarily unique! However
- $\exists!\ H = H(k) = \{f : \mathcal{D} \to \mathbb{R} \text{ functions}\}$ RKHS:
  - $k(\cdot, u) \in H$ $(\forall u \in \mathcal{D})$,
  - $\langle f, k(\cdot, u) \rangle_H = f(u)$ $(\forall u \in \mathcal{D}, \forall f \in H)$.
- In other words,
  - $\varphi(u) := k(\cdot, u)$ is a good choice.
  - $k(\cdot, u)$: represents evaluation.

Some example domains ($\mathcal{D}$), where kernels exist

- Euclidean spaces: $\mathcal{D} = \mathbb{R}^d$.
- Strings, time series, graphs, dynamical systems.

- Distributions.

Distribution kernel: example (used in our work)

- Given: $(\mathcal{D}, k)$; we saw that $u \to \varphi(u) = k(\cdot, u) \in H(k)$.
- Let x be a distribution on $\mathcal{D}$ ($x \in \mathcal{M}_1^+(\mathcal{D})$); the previous construction can be extended:

$$\mu_x = \int_{\mathcal{D}} k(\cdot, u)\mathrm{d}x(u) \in H(k). \tag{1}$$

- If k is bounded: μ_x is well-defined for *any* distribution x.

Mean embedding based distribution kernel

Simple estimation of $\mu_x = \int_{\mathcal{D}} k(\cdot, u)\mathrm{d}x(u)$:

- Empirical distribution: having samples $\{x_n\}_{n=1}^N$

$$\hat{x} = \frac{1}{N}\sum_{n=1}^{N} \delta_{x_n}. \tag{2}$$

- Mean embedding, inner product – empirically:

$$\mu_{\hat{x}} = \int_{\mathcal{D}} k(\cdot, u)\mathrm{d}\hat{x}(u) = \frac{1}{N}\sum_{n=1}^{N} k(\cdot, x_n), \tag{3}$$

$$K\left(\mu_{\hat{x}_i}, \mu_{\hat{x}_j}\right) = \left\langle \mu_{\hat{x}_i}, \mu_{\hat{x}_j} \right\rangle_{H(k)} = \frac{1}{N^2}\sum_{n,m=1}^{N} k(x_{i,n}, x_{j,m}). \tag{4}$$

Mini summary

- Until now
  - If we are given a domain ($\mathcal{D}$) with kernel k, then
  - one can easily define/estimate the similarity of distributions on $\mathcal{D}$.
- Prototype example: $\mathcal{D} = \mathbb{R}^d$, $k =$ Gaussian kernel.

- The *real* conditions:
  - $\mathcal{D}$: LCH + Polish. k: c_0-universal.
  - K: Hölder continuous.

Distribution regression problem: intuitive definition

- $\mathbf{z} = \{(x_i, y_i)\}_{i=1}^{l}$: $x_i \in M_1^+(\mathcal{D})$, $y_i \in \mathbb{R}$.
- $\hat{\mathbf{z}} = \left\{\left(\{x_{i,n}\}_{n=1}^{N}, y_i\right)\right\}_{i=1}^{l}$: $x_{i,1}, \ldots, x_{i,N} \overset{i.i.d.}{\sim} x_i$.
- Goal: learn the relation between x and y based on $\hat{\mathbf{z}}$.
- Idea: embed the distributions (μ) + apply ridge regression

$$M_1^+(\mathcal{D}) \xrightarrow{\mu} X(\subseteq H = H(k)) \xrightarrow{f \in \mathcal{H} = \mathcal{H}(K)} \mathbb{R}.$$

Objective function

- $f_{\mathcal{H}} \in \mathcal{H} = \mathcal{H}(K)$: ideal/optimal in expected risk sense ($\mathcal{E}$):

$$\mathcal{E}\left[f_{\mathcal{H}}\right] = \inf_{f \in \mathcal{H}} \mathcal{E}[f] = \inf_{f \in \mathcal{H}} \int_{X \times \mathbb{R}} [f(\mu_a) - y]^2 \mathrm{d}\rho(\mu_a, y). \qquad (5)$$

- One-stage difficulty ($\int \to \mathbf{z}$):

$$f_{\mathbf{z}}^{\lambda} = \arg\min_{f \in \mathcal{H}} \left(\frac{1}{l} \sum_{i=1}^{l} [f(\mu_{x_i}) - y_i]^2 + \lambda \|f\|_{\mathcal{H}}^2 \right). \qquad (6)$$

- Two-stage difficulty ($\mathbf{z} \to \hat{\mathbf{z}}$):

$$f_{\hat{\mathbf{z}}}^{\lambda} = \arg\min_{f \in \mathcal{H}} \left(\frac{1}{l} \sum_{i=1}^{l} [f(\mu_{\hat{x}_i}) - y_i]^2 + \lambda \|f\|_{\mathcal{H}}^2 \right). \qquad (7)$$

Algorithmically: ridge regression ⇒ simple solution

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

$$(f_{\hat{\mathbf{z}}}^{\lambda} \circ \mu)(t) = [y_1, \ldots, y_l](\mathbf{K} + l\lambda \mathbf{I}_l)^{-1} \begin{bmatrix} K(\mu_{\hat{x}_1}, \mu_t) \\ \vdots \\ K(\mu_{\hat{x}_l}, \mu_t) \end{bmatrix}, \qquad (8)$$

$$\mathbf{K} = [K_{ij}] = [K(\mu_{\hat{x}_i}, \mu_{\hat{x}_j})] \in \mathbb{R}^{l \times l}. \qquad (9)$$

Consistency result

- We studied
  - the excess error: $\mathcal{E}\left[f_{\hat{\mathbf{z}}}^{\lambda}\right] - \mathcal{E}\left[f_{\mathcal{H}}\right]$, i.e,
  - the goodness compared to the best function from $\mathcal{H}$.
- Result: with probability $\to 1$

$$\mathcal{E}\left[f_{\hat{\mathbf{z}}}^{\lambda}\right] - \mathcal{E}\left[f_{\mathcal{H}}\right] \to 0, \tag{10}$$

if we appropriately choose the (l, N, λ) triplet.

Consistency result: $\mathcal{P}(b,c)$ class

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

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

  with eigenvalues t_n $(n = 1, 2, \ldots)$.
- Let $\rho \in \mathcal{P}(b,c)$ be the set of distributions on $X \times \mathbb{R}$:
  - $\alpha \le n^b t_n \le \beta \quad (\forall n \ge 1; \alpha > 0, \beta > 0)$,
  - $\exists g \in \mathcal{H}$ such that $f_{\mathcal{H}} = T^{\frac{c-1}{2}} g$ with $\|g\|_{\mathcal{H}}^2 \le R$ $(R > 0)$,

  where $b \in (1, \infty)$, $c \in [1, 2]$.

Consistency result: an example

- Let $l = N^a$ $(a > 0)$.
- If $\lambda = \left[\frac{\log(N)}{N}\right]^{\frac{1}{c+3}}$ and $\frac{\frac{1}{b}+c}{c+3} \le a$, then with high probability

$$\mathcal{E}\left[f_{\hat{\mathbf{z}}}^{\lambda}\right] - \mathcal{E}\left[f_{\mathcal{H}}\right] \le \mathcal{O}\left(\left[\frac{\log(N)}{N}\right]^{\frac{c}{c+3}}\right) \to 0. \qquad (11)$$

Numerical illustration: supervised entropy learning

- Problem: learn the entropy of Gaussians in a supervised manner.
- Formally:
  - $A = [A_{i,j}] \in \mathbb{R}^{2\times 2}$, $A_{ij} \sim U[0,1]$.
  - 100 sample sets: $\{N(0,\Sigma_u)\}_{u=1}^{100}$, where
    - $100 = 25(\text{training}) + 25(\text{validation}) + 50(\text{testing})$.
    - one set $=$ 500 i.i.d. 2D points,
    - $\Sigma_u = R(\beta_u)AA^T R(\beta_u)^T$,
    - $R(\beta_u)$: 2d rotation,
    - angle $\beta_u \sim U[0,\pi]$.

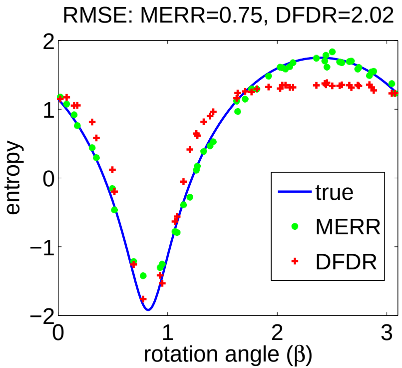
Supervised entropy learning: goal, performance measure

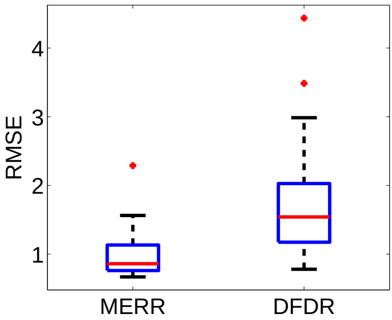
- Goal: learn the entropy of the first marginal

$$H = \frac{1}{2} \ln \left(2\pi e \sigma^2\right), \quad \sigma^2 = M_{1,1}, \quad M = \Sigma_u \in \mathbb{R}^{2\times 2}. \quad (12)$$

- Baseline: kernel smoothing based distribution regression (applying density estimation)
- Performance: RMSE boxplot over 25 random experiments.

Supervised entropy learning: results





Numerical illustration: aerosol prediction

- Bags:
  - randomly selected pixels,
  - within a $20km$ radius around an AOD sensor.
- 800 bags, 100 instances/bag.
- Instances: $x_{i,n} \in \mathbb{R}^{16}$.

Aerosol prediction - baseline

- Baseline: state-of-the-art mixture model
  - EM optimization,
  - $800 = 4 \times 160$(training) $+ 160$(test); 5-fold CV, 10 times (splits).
  - Accuracy: $100 \times RMSE(\pm \text{ std}) = 7.5 - 8.5$ $(\pm 0.1 - 0.6)$.
- Ridge regression:
  - $800 = 3 \times 160$(training) $+ 160$(validation) $+ 160$(test),
  - 5-fold CV, 10 times,
  - validation: λ regularization, θ kernel parameter.

Aerosol prediction: kernel k

- We picked 10 kernels (k): 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).
- We also studied their ensembles.
- Explored parameter domain:

$$(\lambda, \theta) \in \left\{2^{-65}, 2^{-64}, \ldots, 2^{-3}\right\} \times \left\{2^{-15}, 2^{-14}, \ldots, 2^{10}\right\}.$$

- First, K was linear.

Aerosol prediction: kernel definitions

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

$$k_G(a,b) = e^{-\frac{\|a-b\|_2^2}{2\theta^2}}, \qquad k_e(a,b) = e^{-\frac{\|a-b\|_2}{2\theta^2}}, \tag{13}$$

$$k_C(a,b) = \frac{1}{1 + \frac{\|a-b\|_2^2}{\theta^2}}, \quad k_t(a,b) = \frac{1}{1 + \|a-b\|^{\theta}}, \tag{14}$$

$$k_p(a,b) = \left(\langle a,b\rangle + \theta\right)^p, \; k_r(a,b) = 1 - \frac{\|a-b\|_2^2}{\|a-b\|_2^2 + \theta}, \tag{15}$$

$$k_i(a,b) = \frac{1}{\sqrt{\|a-b\|_2^2 + \theta^2}}, \tag{16}$$

$$k_{M,\frac{3}{2}}(a,b) = \left(1 + \frac{\sqrt{3}\,\|a-b\|_2}{\theta}\right) e^{-\frac{\sqrt{3}\|a-b\|_2}{\theta}}, \tag{17}$$

$$k_{M,\frac{5}{2}}(a,b) = \left(1 + \frac{\sqrt{5}\,\|a-b\|_2}{\theta} + \frac{5\,\|a-b\|_2^2}{3\theta^2}\right) e^{-\frac{\sqrt{5}\|a-b\|_2}{\theta}}. \tag{18}$$

Aerosol prediction: results (K: linear)

$100 \times RMSE(\pm std)$ [baseline: $7.5 - 8.5$ $(\pm 0.1 - 0.6)$]:

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

Best combination in the ensemble: $k = k_G, k_C, k_i$.

Aerosol prediction: nonlinear K

- We fed the mean embedding distance ($\|\mu_x - \mu_y\|_{H(k)}$) to the previous kernels.
- Example (RBF on mean embeddings):

$$K(\mu_a, \mu_b) = e^{-\frac{\|\mu_a - \mu_b\|^2_{H(k)}}{2\theta_K^2}} \quad (\mu_a, \mu_b \in X). \tag{19}$$

- We studied the efficiency of (i) single, (ii) ensembles of kernels [(k, K) pairs].

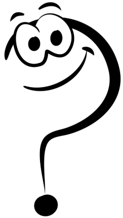
Aerosol prediction: nonlinear K, results

- Baseline:
  - Mixture model (EM): $7.5 - 8.5$ ($\pm 0.1 - 0.6$),
  - Linear K (single): 7.91 ($\pm$1.61).
  - Linear K (ensemble): **7.86** ($\pm$**1.71**).
- Nonlinear K:
  - Single: 7.90 ($\pm$1.63),
  - Ensemble:
    - Accuracy: **7.81** ($\pm$**1.64**),
    - $(k, K) = (k_i, k_t), \left(k_{M,\frac{3}{2}}, k_{M,\frac{3}{2}}\right), (k_C, k_G)$.

Summary

- Problem: distribution regression.
- Difficulty: two-stage sampling.
- Examined solution: ridge regression (simple alg.)!
- Contribution:
  - consistency; convergence rate.
  - submitted to ICML-2014; available on arXiv.
- Code: see the ITE toolbox (`https://bitbucket.org/szzoli/ite/`).

Thank you for the attention!



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