Minimax-optimal Distribution Regression

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Joint work with

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Example: sustainability

- **Goal**: aerosol prediction = air pollution $\rightarrow$ climate.

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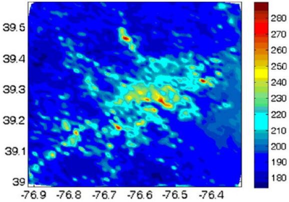
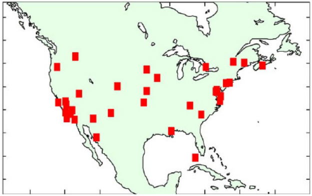
- Prediction using labelled bags:
  - bag := multi-spectral satellite measurements over an area,
  - label := local aerosol value.

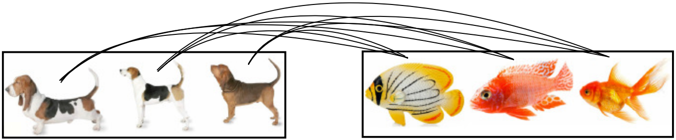




Example: existing methods

Multi-instance learning:

- [Haussler, 1999, Gärtner et al., 2002] (set kernel):



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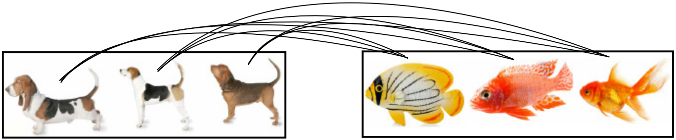

- sensible methods in regression: few,
  1. restrictive technical conditions,
  2. super-high resolution satellite image: would be needed.

One-page summary

Contributions:

1. Practical: state-of-the-art accuracy (aerosol).
2. Theoretical:
   - General bags: graphs, time series, texts, ...
   - Consistency of set kernel in regression (17-year-old open problem).
   - How many samples/bag?

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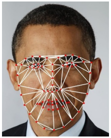
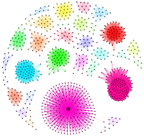
Objects in the bags





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  - network analysis: group of people = bag of friendship graphs, ...

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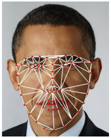

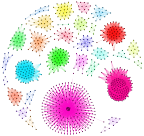

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- Wider context (statistics): point estimation tasks.

Regression on labelled bags

- Given:
  - labelled bags: $\hat{\mathbf{z}} = \left\{\left(\hat{P}_i, y_i\right)\right\}_{i=1}^{\ell}$, $\hat{P}_i$: bag from P_i, $N := |\hat{P}_i|$.
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- Estimator:

$$f_{\hat{\mathbf{z}}}^{\lambda} = \arg\min_{f \in \mathcal{H}} \frac{1}{\ell} \sum_{i=1}^{\ell} \left[f\underbrace{\left(\mu_{\hat{P}_i}\right)}_{\text{feature of } \hat{P}_i} - y_i \right]^2 + \lambda \|f\|_{\mathcal{H}}^2 .$$

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- Prediction:

$$\hat{y}\left(\hat{P}\right) = \mathbf{g}^T (\mathbf{G} + \ell\lambda\mathbf{I})^{-1}\mathbf{y},$$
$$\mathbf{g} = \left[K\left(\mu_{\hat{P}}, \mu_{\hat{P}_i}\right)\right], \mathbf{G} = \left[K\left(\mu_{\hat{P}_i}, \mu_{\hat{P}_j}\right)\right], \mathbf{y} = [y_i].$$

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Challenges

1. Inner product of distributions: $K\left(\mu_{\hat{P}_i}, \mu_{\hat{P}_j}\right) = ?$
2. How many samples/bag?

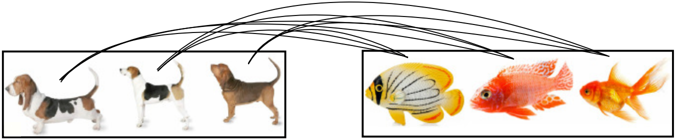
Regression on labelled bags: similarity

Let us define an inner product on distributions $[\tilde{K}(P,Q)]$:

1. Set kernel: $A = \{a_i\}_{i=1}^N$, $B = \{b_j\}_{j=1}^N$.

$$\tilde{K}(A,B) = \frac{1}{N^2}\sum_{i,j=1}^{N} k(a_i,b_j) = \left\langle \underbrace{\frac{1}{N}\sum_{i=1}^{N}\varphi(a_i)}_{\text{feature of bag } A}, \frac{1}{N}\sum_{j=1}^{N}\varphi(b_j) \right\rangle.$$

Remember:



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2. Taking 'limit' [Berlinet and Thomas-Agnan, 2004, Altun and Smola, 2006, Smola et al., 2007]: $a \sim P, b \sim Q$

$$\tilde{K}(P,Q) = \mathbb{E}_{a,b}k(a,b) = \left\langle \underbrace{\mathbb{E}_a\varphi(a)}_{\text{feature of distribution } P =: \mu_P}, \mathbb{E}_b\varphi(b) \right\rangle.$$

Example (Gaussian kernel): $k(\mathbf{a},\mathbf{b}) = e^{-\|\mathbf{a}-\mathbf{b}\|_2^2/(2\sigma^2)}$.

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- $k : \mathcal{D} \times \mathcal{D} \to \mathbb{R}$ sym. is pd. if $\mathbf{G} = [k(x_i, x_j)]_{i,j=1}^n \succeq 0$.

Kernel examples on $\mathcal{D} = \mathbb{R}^d$, $\theta > 0$

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

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

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

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

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

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

Regression on labelled bags: baseline

Quality of estimator, baseline:

$$\mathcal{R}(f) = \mathbb{E}_{(\mu_P, y)\sim\rho}[f(\mu_P) - y]^2,$$
$$f_\rho = \text{best regressor}.$$

How many samples/bag to get the accuracy of f_ρ? Possible?

Assume (for a moment): $f_\rho \in \mathcal{H}(K)$.

Our result: how many samples/bag

- Known [Caponnetto and De Vito, 2007]: best/achieved rate

$$\mathcal{R}(f_{\mathbf{z}}^{\lambda}) - \mathcal{R}(f_{\rho}) = \mathcal{O}\left(\ell^{-\frac{bc}{bc+1}}\right),$$

b – size of the input space, c – smoothness of f_{ρ}.

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- Let $N = \tilde{\mathcal{O}}(\ell^{a})$. N: size of the bags. ℓ: number of bags.

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- If $2 \leq a$, then $f_{\hat{\mathbf{z}}}^{\lambda}$ attains the best achievable rate.
- In fact, $a = \frac{b(c+1)}{bc+1} < 2$ is enough.
- Consequence: regression with set kernel is consistent.

Well-specified case: computational & statistical tradeoff

Let $N = \tilde{\mathcal{O}}\left(\ell^a\right)$.

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- If $\frac{b(c+1)}{bc+1} \leq a$, then $\mathcal{R}\left(f_{\hat{\mathbf{z}}}^{\lambda}\right) - \mathcal{R}\left(f_\rho\right) = \mathcal{O}\left(\ell^{-\frac{bc}{bc+1}}\right)$.

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Meaning:

- smaller a: computational saving, but reduced statistical efficiency.

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Meaning:

- smaller a: computational saving, but reduced statistical efficiency.
- $c \mapsto \frac{b(c+1)}{bc+1}$ decreasing: easier problems $\Rightarrow$ smaller bags.

Why can we get consistency/rates? – intuition

- Convergence of the mean embedding:

$$\left\|\mu_P - \mu_{\hat{P}}\right\|_H = \mathcal{O}\left(\frac{1}{\sqrt{N}}\right).$$

- Hölder property of K ($0 < L$, $0 < h \leq 1$):

$$\left\|K(\cdot,\mu_P) - K(\cdot,\mu_{\hat{P}})\right\|_{\mathcal{H}} \leq L \left\|\mu_P - \mu_{\hat{P}}\right\|_H^h.$$

- $f_{\hat{z}}^{\lambda}$ depends 'nicely' on $\mu_{\hat{P}}$.

Valid similarities

Recall: $K(P,Q) = \langle \mu_P, \mu_Q \rangle$.

K_G	K_e	K_C
$e^{-\frac{\left\|\mu_P-\mu_Q\right\|^2}{2\theta^2}}$	$e^{-\frac{\left\|\mu_P-\mu_Q\right\|}{2\theta^2}}$	$\left(1+\left\|\mu_P-\mu_Q\right\|^2/\theta^2\right)^{-1}$

K_t	K_i
$\left(1+\left\|\mu_P-\mu_Q\right\|^\theta\right)^{-1}$	$\left(\left\|\mu_P-\mu_Q\right\|^2+\theta^2\right)^{-\frac{1}{2}}$

Functions of $\left\|\mu_P-\mu_Q\right\| \Rightarrow$ computation: similar to set kernel.

Extensions

1. Misspecified setting ($f_\rho \in L^2 \backslash \mathcal{H}$):
   - Consistency: convergence to $\inf_{f \in \mathcal{H}} \|f - f_\rho\|_{L^2}$.
   - Smoothness on f_ρ: computational & statistical tradeoff.

Extensions

2. Vector-valued output:
   - Y: separable Hilbert space $\Rightarrow K(\mu_P, \mu_Q) \in \mathcal{L}(Y)$.
   - Prediction on a test bag $\hat{P}$:

$$\hat{y}(\hat{P}) = \mathbf{g}^T(\mathbf{G} + \ell\lambda\mathbf{I})^{-1}\mathbf{y},$$
$$\mathbf{g} = [K(\mu_{\hat{P}}, \mu_{\hat{P}_i})], \mathbf{G} = [K(\mu_{\hat{P}_i}, \mu_{\hat{P}_j})], \mathbf{y} = [y_i].$$

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

Misspecified case: consistency

Our result

Let

- $N = \tilde{\mathcal{O}}(\ell)$,
- $\ell \to \infty$, $\lambda \to 0$, $\lambda\sqrt{\ell} \to \infty$.

Then,

$$\mathcal{R}\left(f_{\hat{\mathbf{z}}}^{\lambda}\right) - \mathcal{R}(f_{\rho}) \to \inf_{f \in \mathcal{H}} \|f - f_{\rho}\|_{L^2}.$$

Misspecified case: s-smooth

Let $N = \tilde{O}\left(\ell^{2a}\right)$. f_ρ: s-smooth, $s \in (0,1]$.

Our result (computational & statistical tradeoff)

- If $\frac{s+1}{s+2} \leq a$, then $\mathcal{R}\left(f_{\hat{\mathbf{z}}}^{\lambda}\right) - \mathcal{R}\left(f_\rho\right) = \mathcal{O}\left(\ell^{-\frac{2s}{s+2}}\right)$.

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- $s \mapsto \frac{2s}{s+2}$ is increasing: easier task = better rate.
    - $s \to 0$: arbitrary slow rate. $s = 1$: $\mathcal{O}(\ell^{-\frac{2}{3}})$ speed.

Misspecified case: optimality

- Our rate: $r(\ell) = \ell^{-\frac{2s}{s+2}}$.
- One-stage sampled optimal rate: $r_o(\ell) = \ell^{-\frac{2s}{2s+1}}$ [Steinwart et al., 2009],
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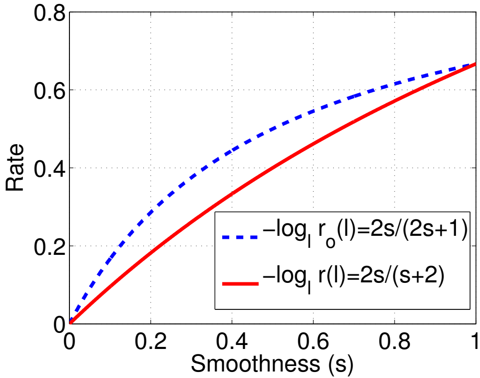

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- General C:

$$C(v) = \sum_n \lambda_n \langle u_n, v\rangle u_n,$$

$$C^s(v) = \sum_n \lambda_n^s \langle u_n, v\rangle u_n,$$

$$Im(C^s) = \left\{\sum_n c_n u_n : \sum_n c_n^2 \lambda_n^{-2s} < \infty\right\}.$$

Larger $s \Rightarrow$ faster decay of the c_n Fourier coefficients.

Aerosol prediction result ($100 \times RMSE$)

We perform on par with the state-of-the-art, hand-engineered method.

- Zhuang Wang, Liang Lan, Slobodan Vucetic. IEEE Transactions on Geoscience and Remote Sensing, 2012: $7.5 - 8.5$ ($\pm 0.1 - 0.6$):
  - hand-crafted features.
- Our prediction accuracy: 7.81 (± 1.64).
  - no expert knowledge.
- Code in ITE: #2 on mloss,

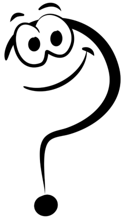
```
https://bitbucket.org/szzoli/ite/
```

Summary

- Problem: distribution regression.
- Contribution:
  - computational & statistical tradeoff analysis,
  - set kernel: ✓
  - minimax optimal rate.

Learning Theory for Distribution Regression. Journal of Machine Learning Research, 17(152):1-40, 2016.

Thank you for the attention!



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