Distribution Regression

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Joint work with

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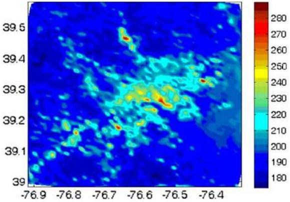
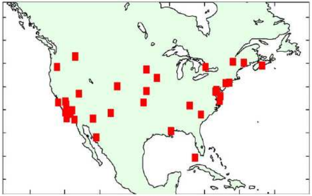
Example: sustainability

- **Goal**: aerosol prediction $\rightarrow$ climate.

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

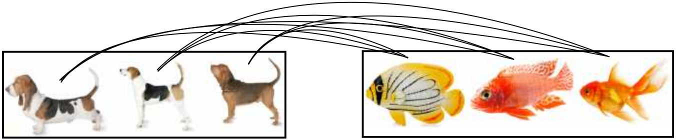




Example: existing methods

Multi-instance learning:

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



- 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? → [Szabó et al., 2016].

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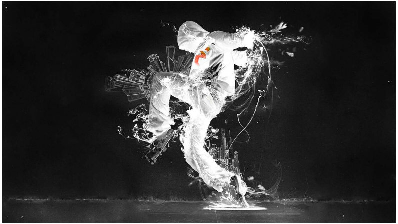
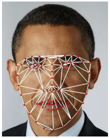
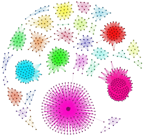


Objects in the bags





- time-series modelling: user = set of time-series,
- computer vision: image = collection of patch vectors,
- NLP: corpus = bag of documents,
- network analysis: group of people = bag of friendship graphs, ...

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, $N := |\hat{P}_i|$.
  - test bag: $\hat{P}$.

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- Estimator:

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

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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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Challenge

How many samples/bag?

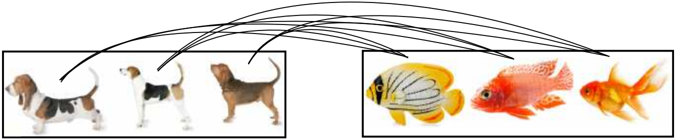
Regression on labelled bags: similarity

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

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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Our result

- 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.

Extensions

1. K: linear $\to$ Hölder, e.g. RBF [Christmann and Steinwart, 2010].

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1. K: linear $\to$ Hölder, e.g. RBF [Christmann and Steinwart, 2010].
2. 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.

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

Aerosol prediction result ($100 \times RMSE$)

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

- [Wang et al., 2012]: 7.5 – 8.5:
  - hand-crafted features.
- Our prediction accuracy: 7.81:
  - no expert knowledge.
- Code in ITE:

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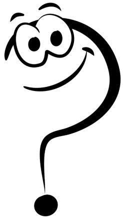
Summary

- Problem: distribution regression.
- Contribution:
  - computational & statistical tradeoff analysis,
  - specifically, the set kernel is consistent,
  - minimax optimal rate is achievable: sub-quadratic bag size.
- Open question: optimal bag size.

Thank you for the attention!



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Altun, Y. and Smola, A. (2006).
Unifying divergence minimization and statistical inference via convex duality.
In *Conference on Learning Theory (COLT)*, pages 139–153.

Berlinet, A. and Thomas-Agnan, C. (2004).
Reproducing Kernel Hilbert Spaces in Probability and Statistics.
Kluwer.

Caponnetto, A. and De Vito, E. (2007).
Optimal rates for regularized least-squares algorithm.
Foundations of Computational Mathematics, 7:331–368.

Christmann, A. and Steinwart, I. (2010).
Universal kernels on non-standard input spaces.
In *Advances in Neural Information Processing Systems (NIPS)*, pages 406–414.

Gärtner, T., Flach, P. A., Kowalczyk, A., and Smola, A. (2002).

Multi-instance kernels.
In *International Conference on Machine Learning (ICML)*, pages 179–186.

Haussler, D. (1999).
Convolution kernels on discrete structures.
Technical report, Department of Computer Science, University of California at Santa Cruz.
(http://cbse.soe.ucsc.edu/sites/default/files/convolutions.pdf).

Smola, A., Gretton, A., Song, L., and Schölkopf, B. (2007).
A Hilbert space embedding for distributions.
In *Algorithmic Learning Theory (ALT)*, pages 13–31.

Szabó, Z., Sriperumbudur, B., Póczos, B., and Gretton, A. (2016).
Learning theory for distribution regression.
Journal of Machine Learning Research, 17(152):1–40.

Wang, Z., Lan, L., and Vucetic, S. (2012).

Mixture model for multiple instance regression and applications in remote sensing.
IEEE Transactions on Geoscience and Remote Sensing, 50:2226–2237.