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 $MMD_{\mathscr{H}}(\mathcal{Q}, \mathcal{P}) := \sup_{\|f\|_{\mathscr{H}} \le 1} \int f d(\mathcal{Q} - \mathcal{P})$ $= \mathbb{E}_{x, x' \sim \mathcal{Q}} k(x, x') + \mathbb{E}_{y, y' \sim \mathcal{P}} k(y, y')$

 $-2\mathbb{E}_{x\sim 0, y\sim P}k(x, y)$

$\sim P$ —	▶ (
$\sim Q$ $\int \phi dP = \mu$	•



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- We can bound performance under Q ($\neq P_0$) beyond statistical fluctuation (classical learning theory)
- Question: how do we actually solve an MMDconstrained optimization problem? (Non-trivial!)







Primal DRO (not solvable as it is)

(DRO) min sup $\mathbb{E}_{Q}l(\theta,\xi)$ $\stackrel{\sim}{\underset{\sim}{\longrightarrow}} \sim Q$



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Kernel DRO Theorem (simplified). [Z. et al. AISTATS 2021] DRO problem is equivalent to the a dual kernel learning problem, i.e., (DRO)=(K).

(K)
$$\min_{\theta, f \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^{N} f(\xi_i) + \epsilon \|f\|_{\mathcal{H}} \text{ subject to } l(\theta, \cdot) \leq \epsilon$$

cf. Kantorovich duality in optimal transport (OT) and Moreau-Yosida regularization in convex analysis

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 Extension to more general ambiguity geometry $\min_{\theta, f \in \mathcal{H}} \delta^*_{\mu(\mathcal{M})}(f) \quad \text{subject to } l(\theta, \cdot) \leq f.$ $\delta^*_{\!\mathscr{C}}$ denotes the support function of the set \mathscr{C}



Many alg. as special cases, e.g., SVM, multi-kernel...

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- Decision variable *f* can be interpreted as the test function in the kernel two-sample test
- Comparison with Wasserstein DRO:
- MMD enjoys closed-form estimator for fast computation and favorable convergence rate
- For general ML loss $l(\theta, \cdot)$ with nonlinear models, there exists no exact reformulation of Wasserstein DRO. Kernel DRO can be applied in such cases thanks to the universality of RKHSs.



Example. Certified adversarially robust learning (Classify the presence of glasses)

















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Recall: Kernel DRO Theorem: (K) $\min_{\theta, f \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^{N} f(\xi_i) + \epsilon ||f||_{\mathcal{H}}$ subject to $l(\theta, \cdot) \leq f$





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Distributional robustness certificate. $\mathcal{W}_{c}(\cdot, \cdot)$: OT metric with transport cost c $\epsilon_N \rightarrow 0$, computable robustness certificate: $\sup_{\mathcal{U}_{c}(Q,P_{0})\leq\rho} \mathbb{E}_{Q} \ln l(\hat{\theta},\xi)$ $\leq \ln \left\{ \frac{1}{N} \sum_{i=1}^{N} \sup_{z} \left\{ l(\hat{\theta}, z) k(z, \xi_{i}) \right\} \right\} + \frac{\rho}{\sigma} + \epsilon_{N}$

ARKS objective



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Interesting future directions

- Design specific kernels for robustness beyond normball perturbation
- Physics, information geometry, and general dynamic OT
- Causal inference via distributional robustness

References

- **Zhu**, J.-J., Jitkrittum, W., Diehl, M. & Schölkopf, B. Kernel Distributionally Robust Optimization. AISTATS 2021
- **Zhu**, J.-J., Kouridi, C., Nemmour, Y. & Schölkopf, B. Adversarially Robust Kernel Smoothing. AISTATS 2022

Code

- KDRO: <u>https://github.com/jj-zhu/kdro</u>
- ARKS: <u>https://github.com/christinakouridi/arks</u>



Website: <u>jj-zhu.github.io</u>