# Duality from Distributionally Robust Learning to Gradient Flow Force-Balance

Jia-Jie Zhu

Weierstrass Institute for Applied Analysis and Stochastics, Berlin

jj-zhu.github.io

Weierstraß-Institut für
Angewandte Analysis und Stochastik

Based on previous and on-going work with
students and collaborators

DP4ML Workshop, ICML 2023
Honolulu Hawaii, USA, July, 2023,

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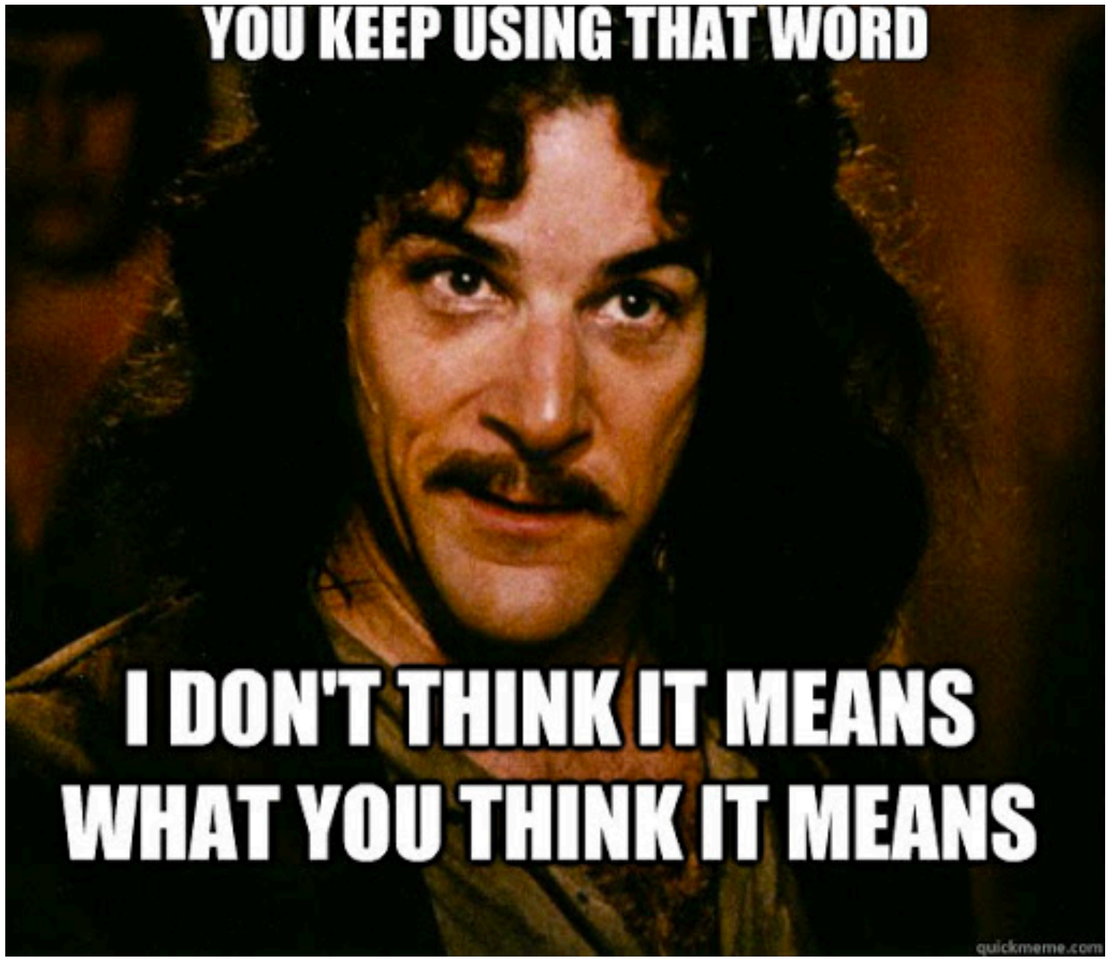


Figure credit: The Princess Bride,
a bedside story by your grandpa

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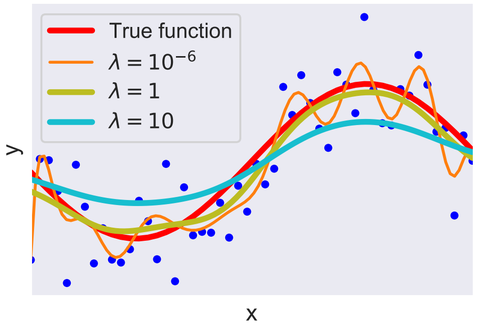

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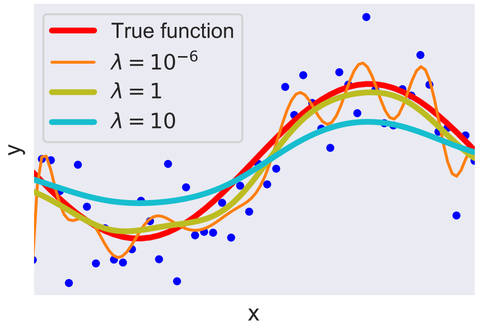


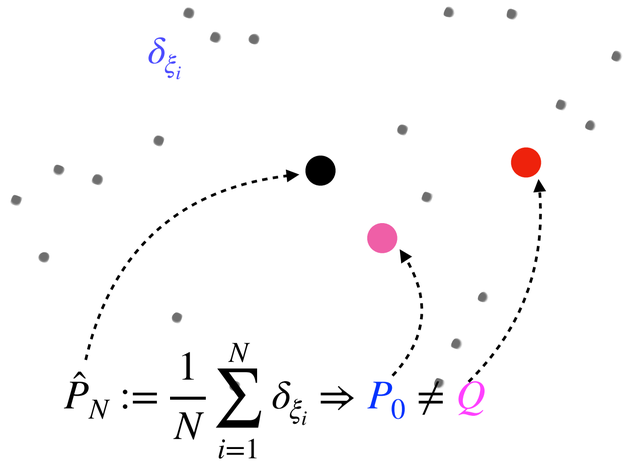

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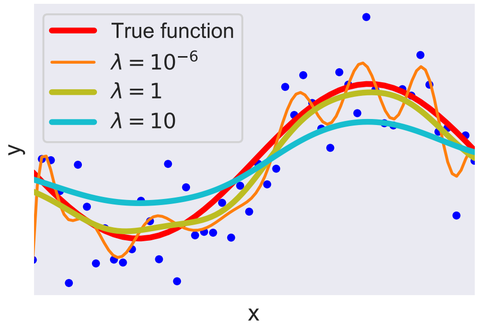


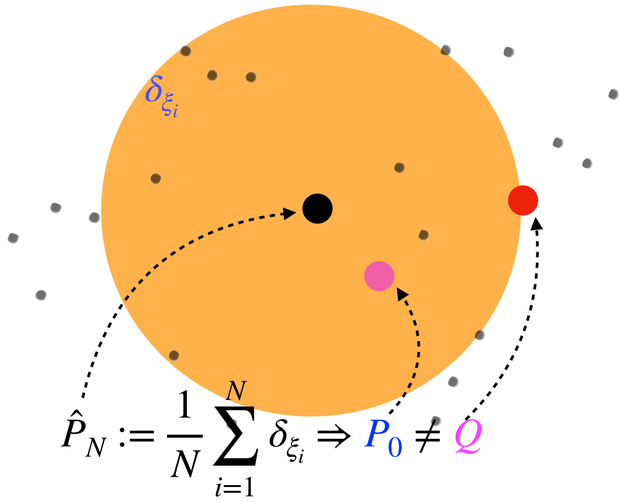


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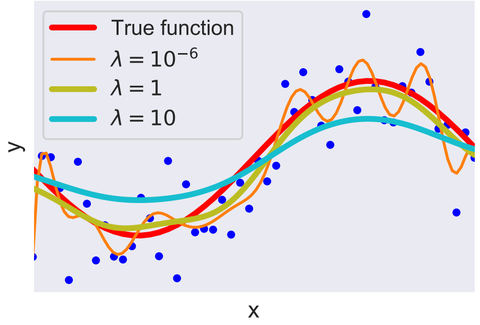


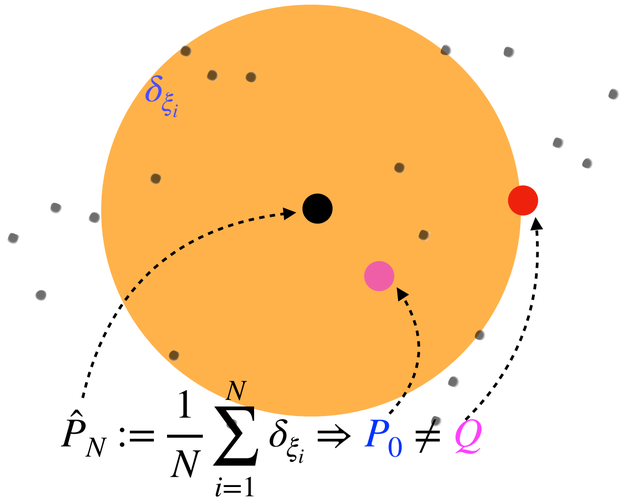


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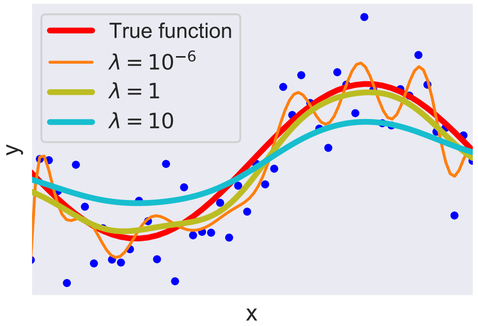


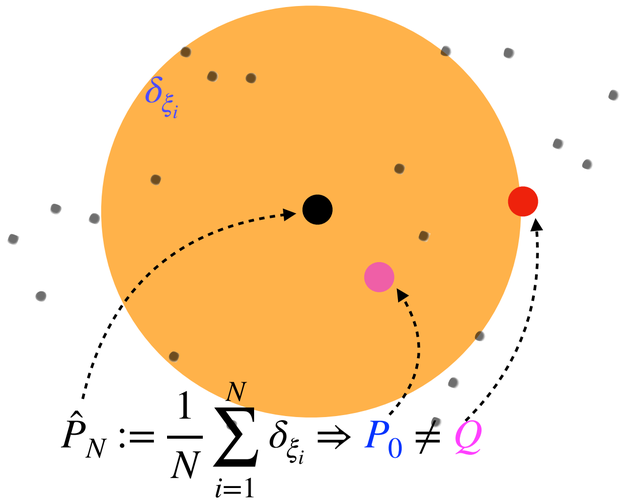


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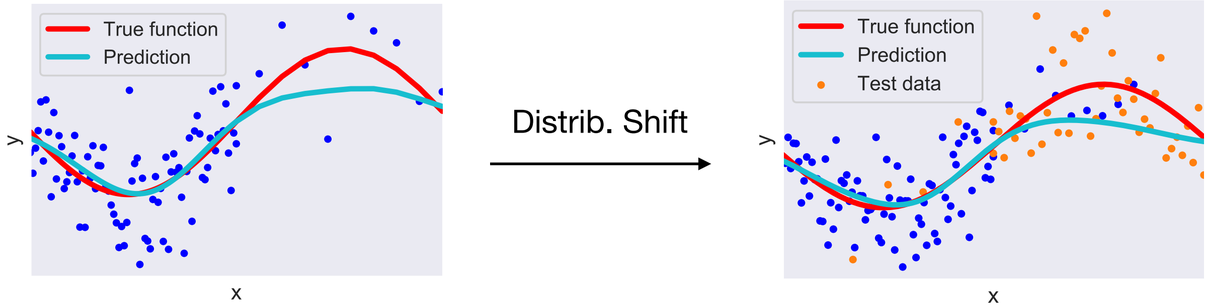


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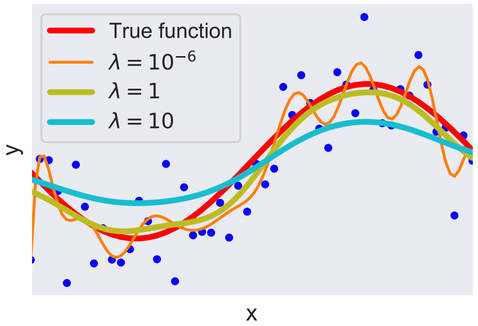


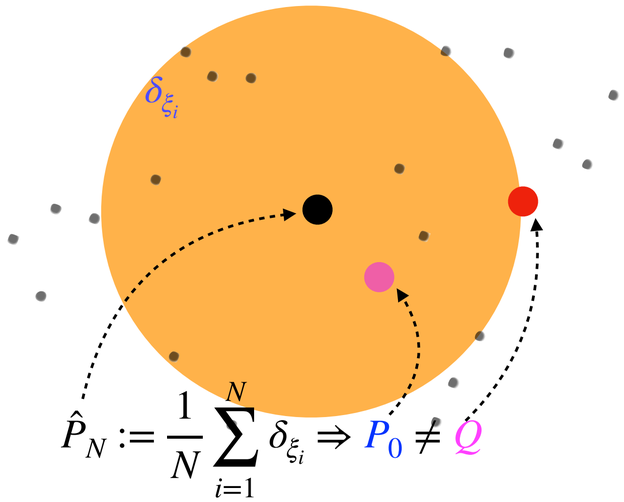


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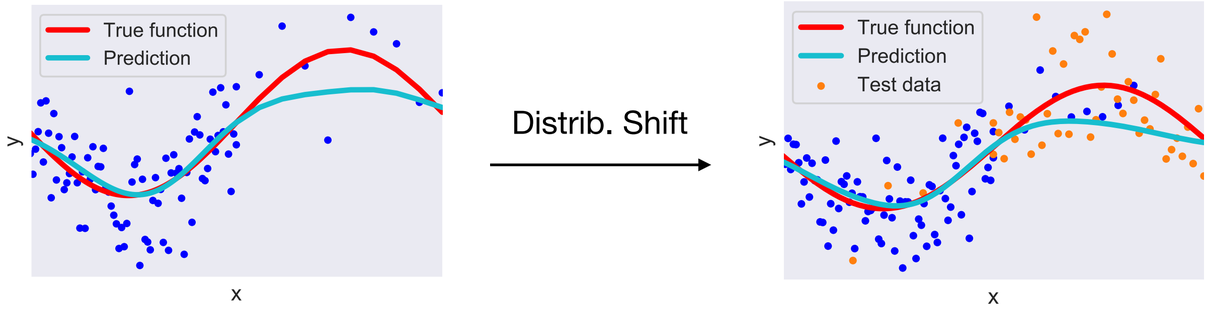


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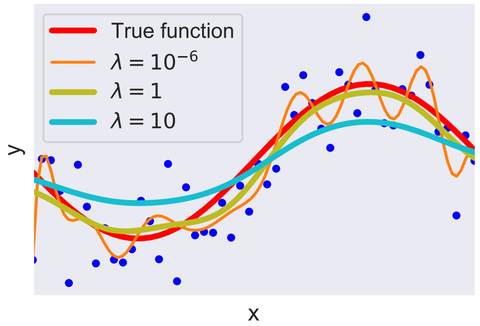


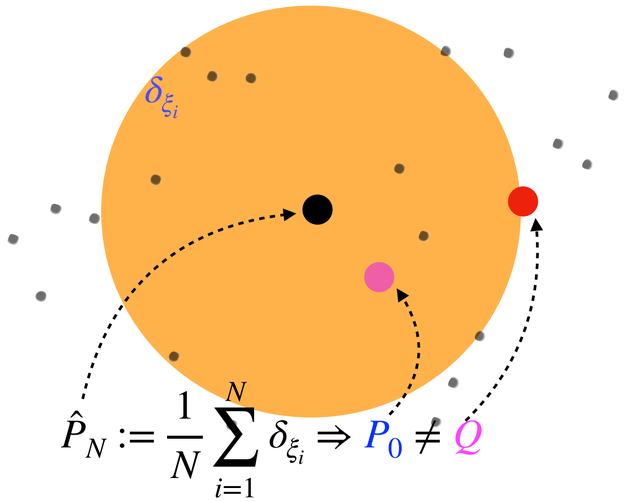


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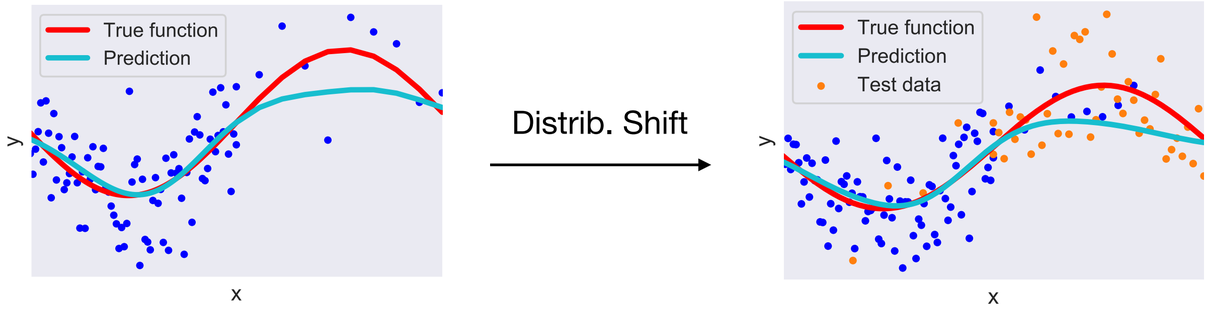


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New geometries leading to new fields of research and breakthroughs:

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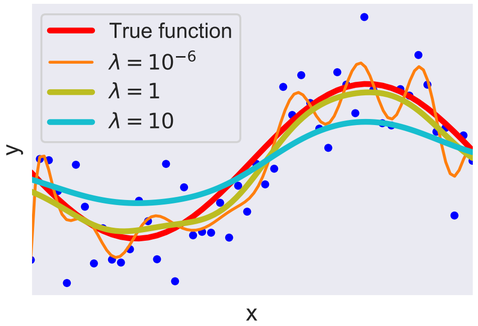


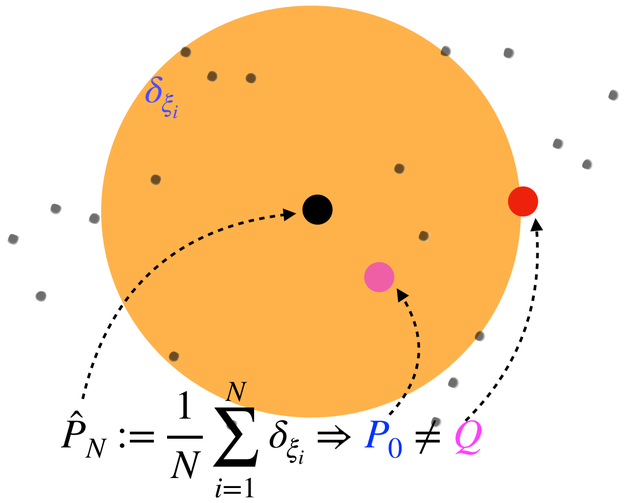


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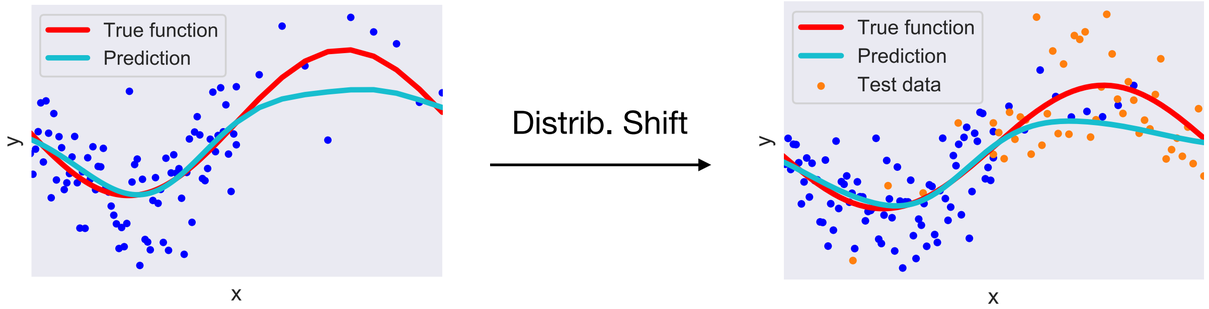


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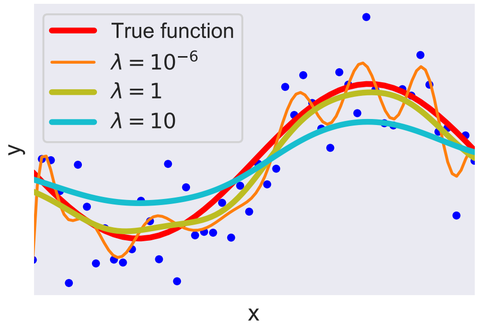


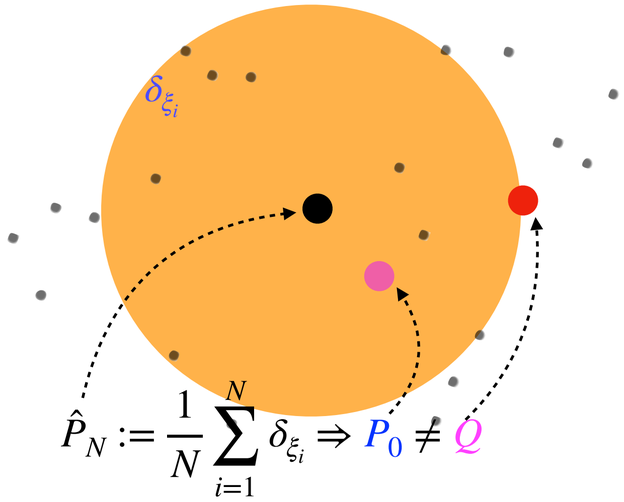


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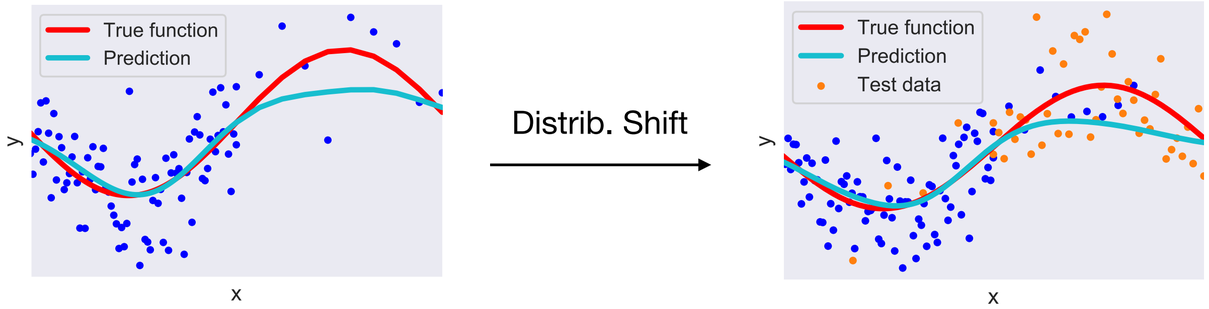


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**Wasserstein Gradient flow** [F. Otto et al.] e.g. Fokker-Planck equation as GF in W2

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**Definition.** The $p$**-Wasserstein distance** between probability measures $P, Q$ on $\mathbb{R}^d$ (with $p$ finite moments, $p \geq 1$) is defined through the following Kantorovich problem

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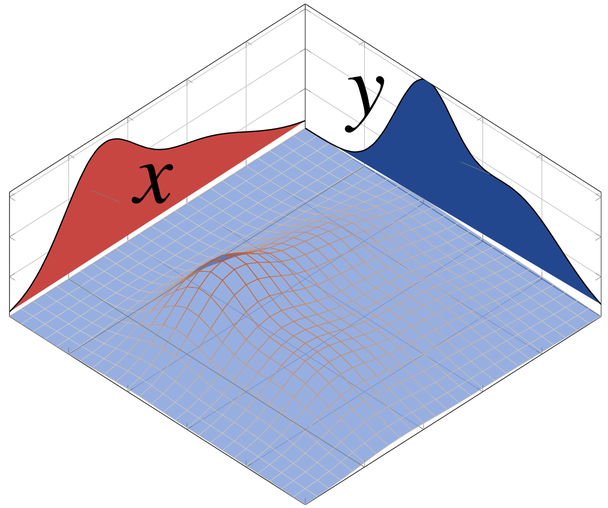

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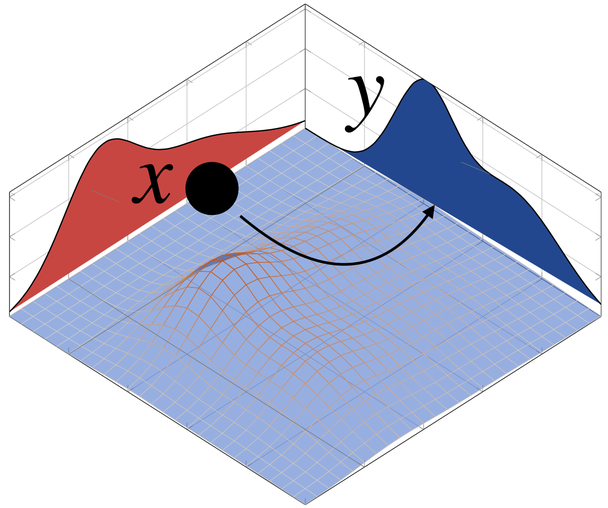

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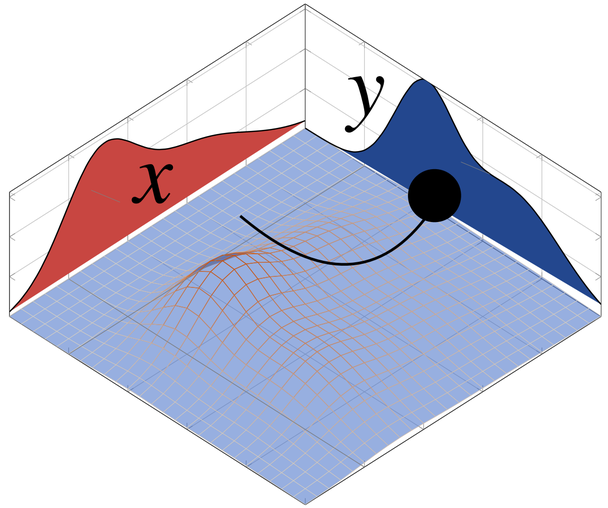

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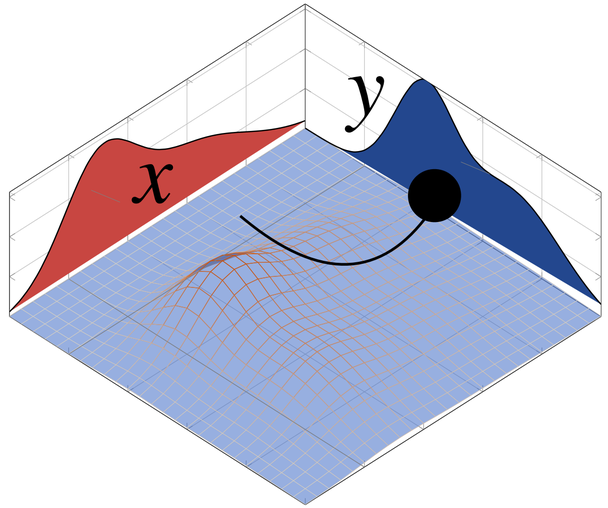


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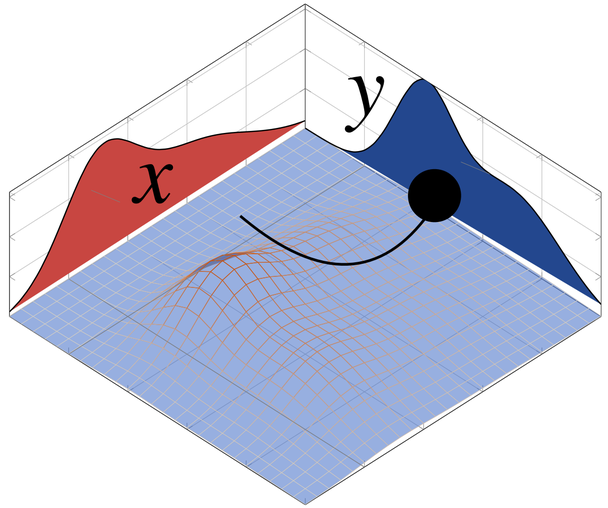


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**Dynamic formulation:** ***Benamou–Brenier***

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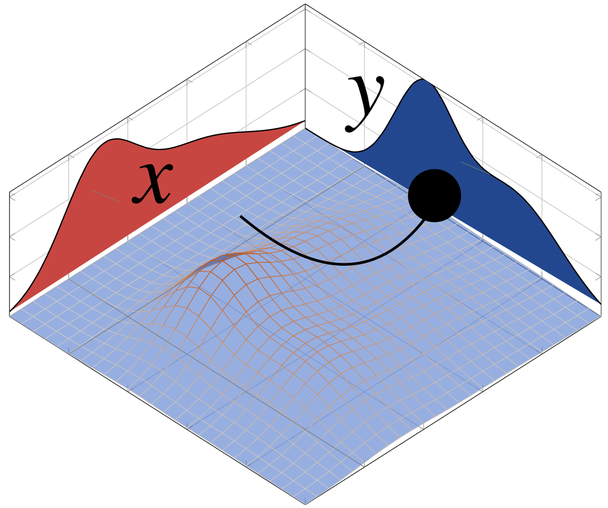


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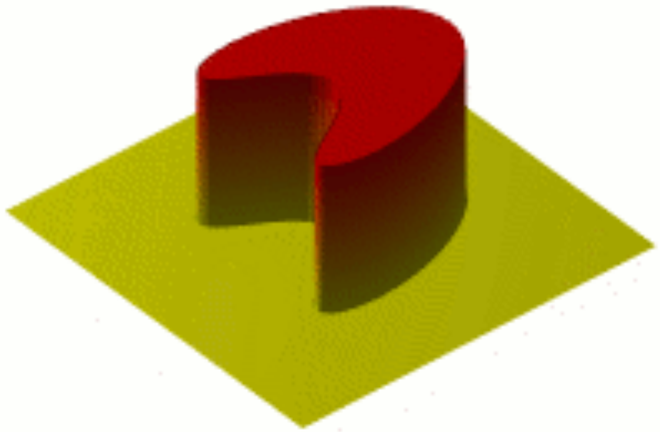

# Background: “Kernel Geometry”

Figure credit: W. Jitkrittum, J. Zhu

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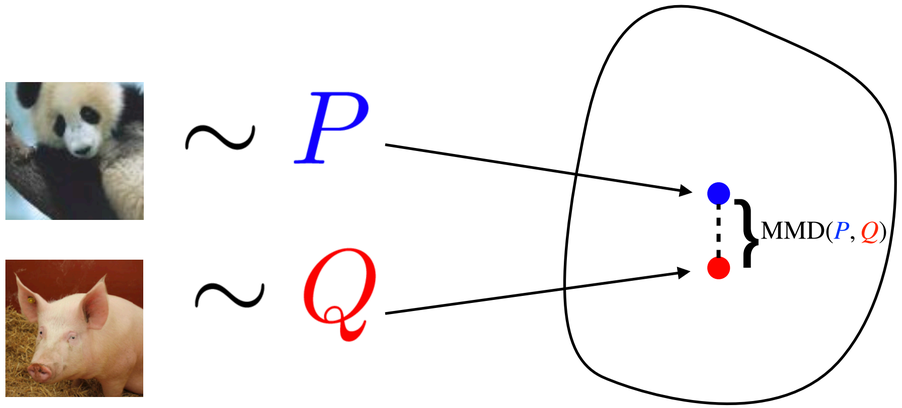
**Definition.** Kernel **Maximum-Mean Discrepancy** (MMD) associated with (PSD) kernel $k$ (e.g., $k(x, x') := e^{-|x-x'|^2/\sigma}$)

$$\mathrm{MMD}(P, Q) := \left\| \int k(x, \cdot)\, dP - \int k(x, \cdot)\, dQ \right\|_{\mathscr{H}}.$$

$(\mathrm{Prob}(\mathbb{R}^d), \mathrm{MMD})$ is a (simple) metric space.

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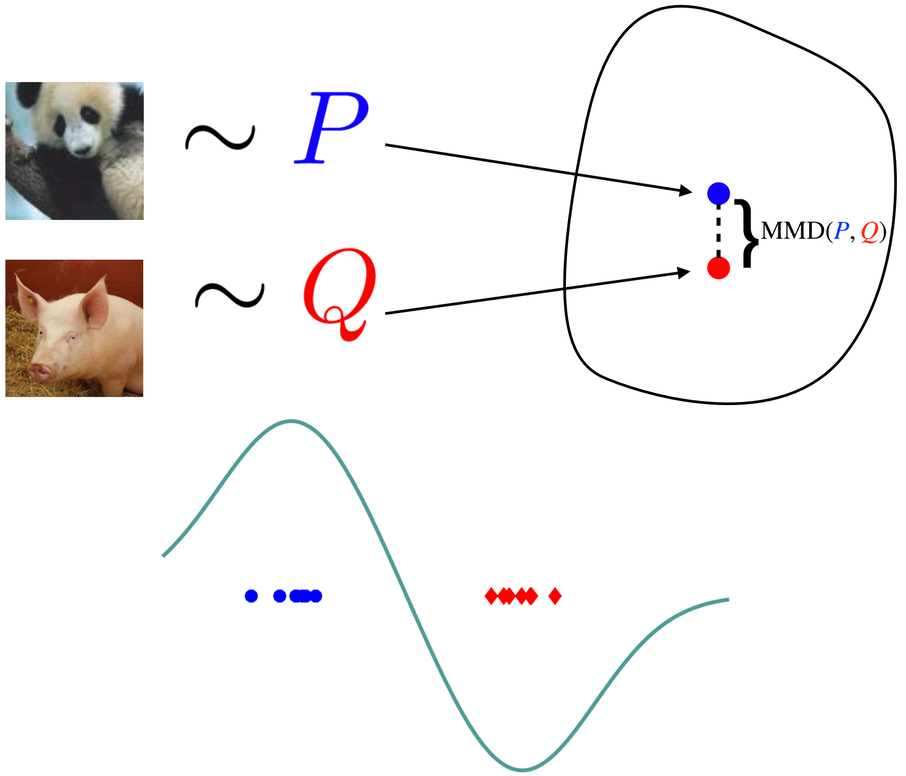
$$\mathrm{MMD}(P, Q) = \sup_{\|f\|_{\mathscr{H}} \le 1} \int f\, d(P - Q)$$

$\mathscr{H}$ is the **reproducing kernel Hilbert space** $\mathscr{H}$ (RKHS), which satisfies $f(x) = \langle f, \phi(x) \rangle_{\mathscr{H}}, \forall f \in \mathscr{H}, x \in \mathscr{X}$, $\phi(x) := k(x, \cdot)$ is the canonical feature of $\mathscr{H}$.

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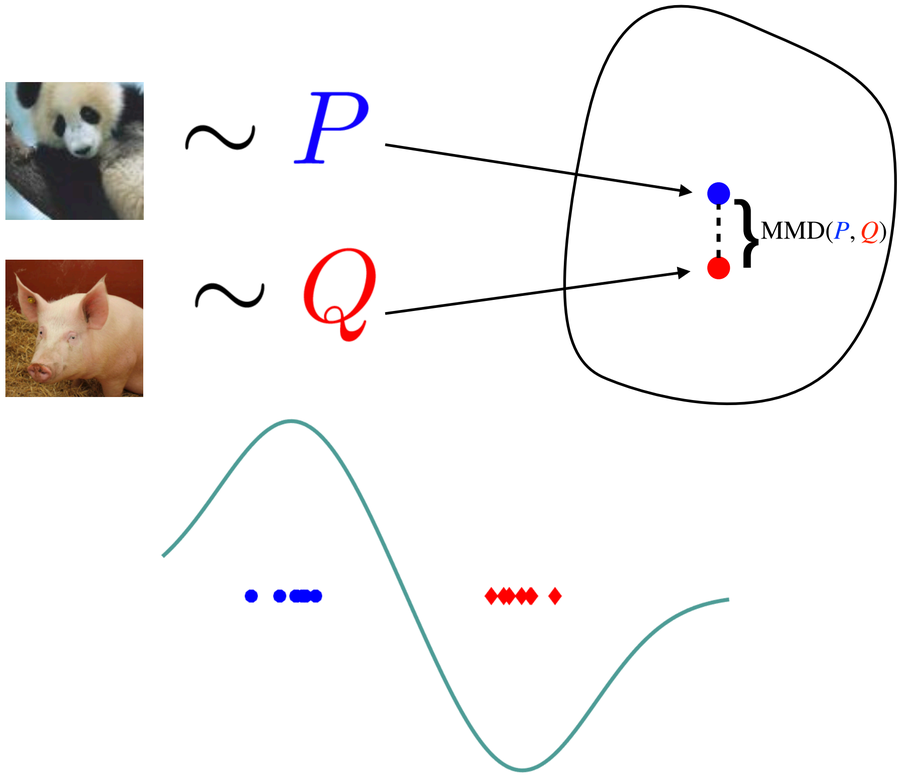


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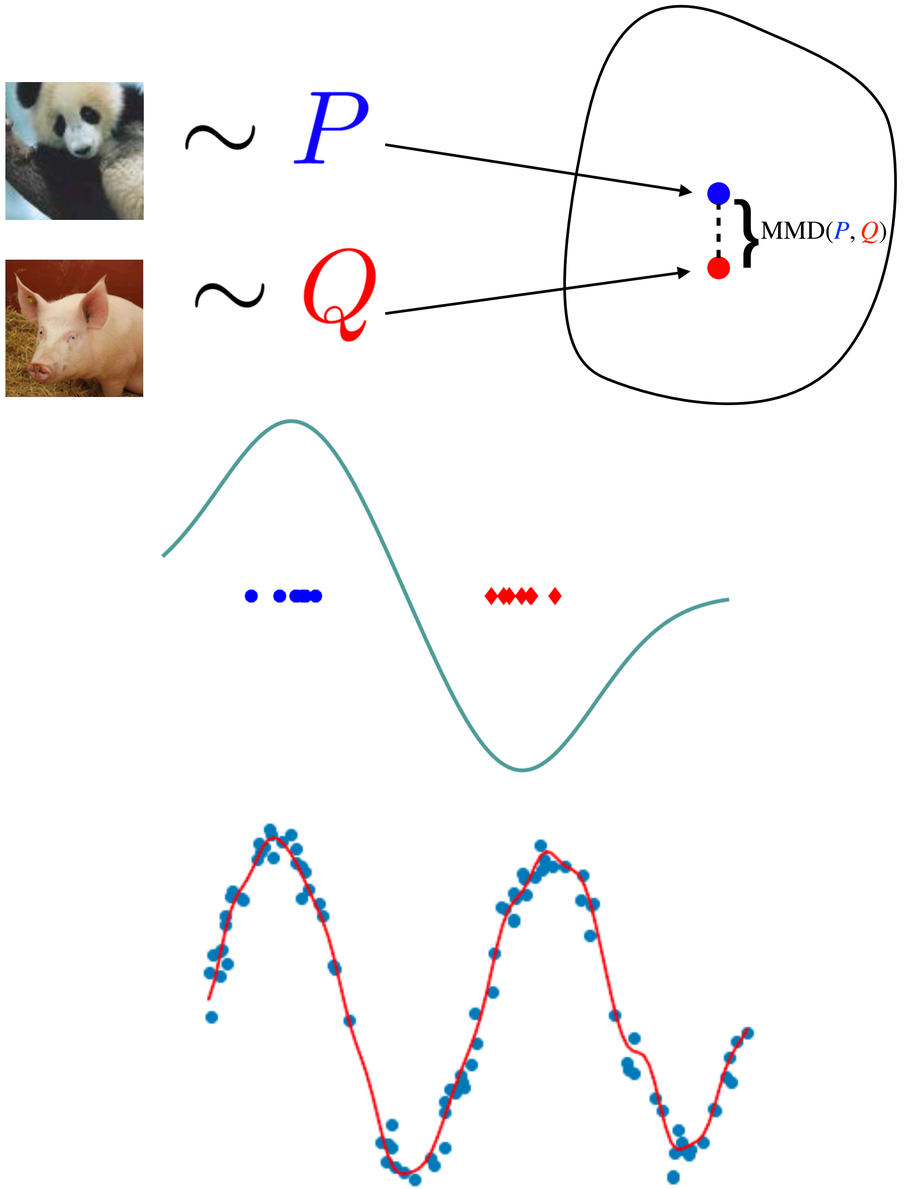


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# Kernel distributionally robust optimization

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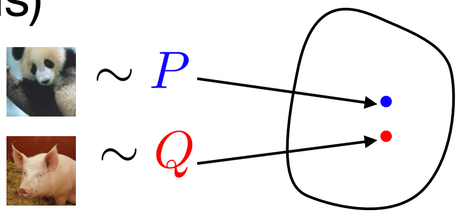
**Primal DRO** (not solvable as it is)

$$\text{(DRO)} \quad \min_{\theta} \sup_{\mathrm{MMD}(Q,\hat{P})\leq\epsilon} \mathbb{E}_{Q} l(\theta, \xi)$$



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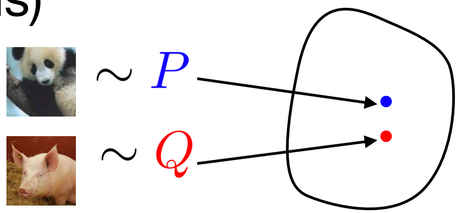


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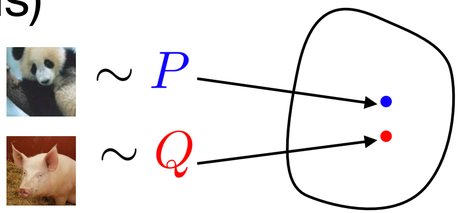


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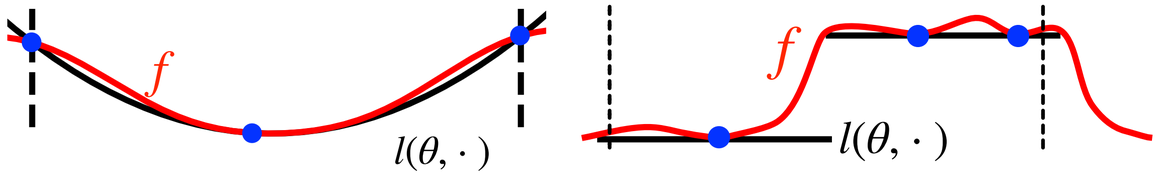

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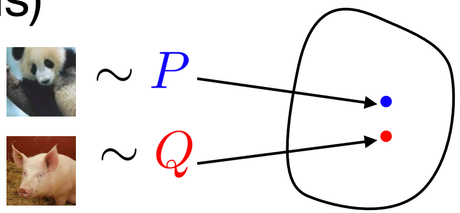


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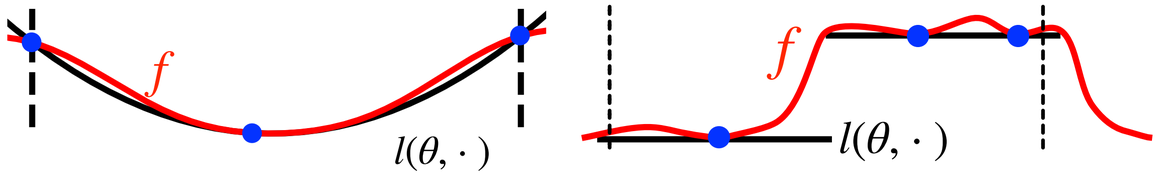


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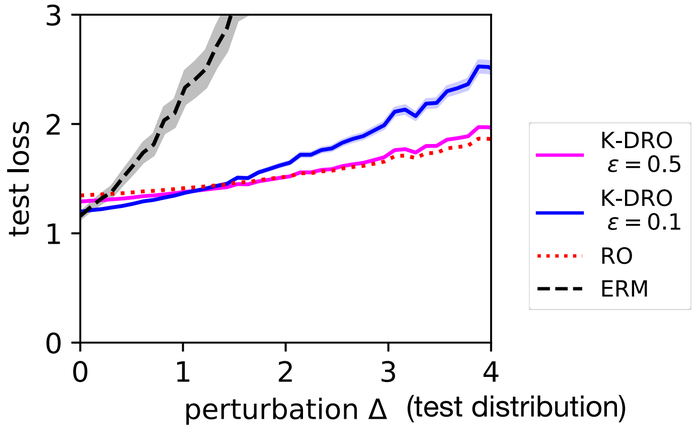

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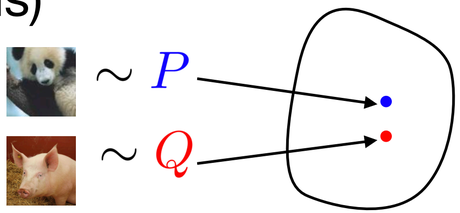


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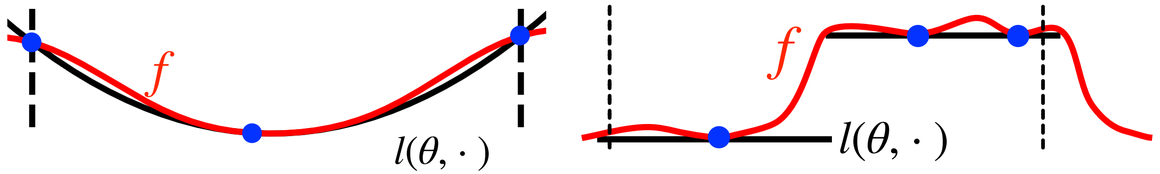


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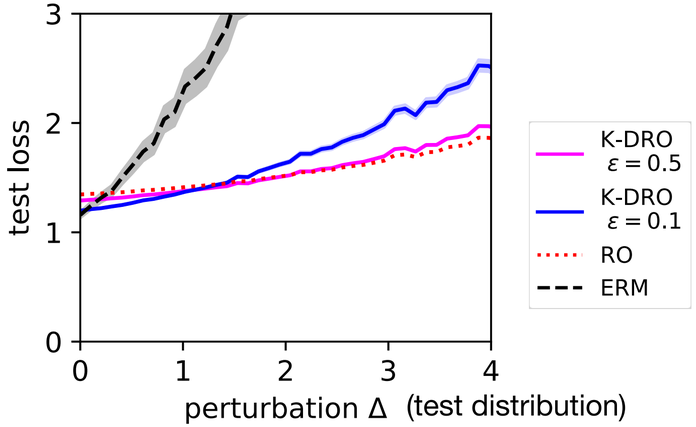


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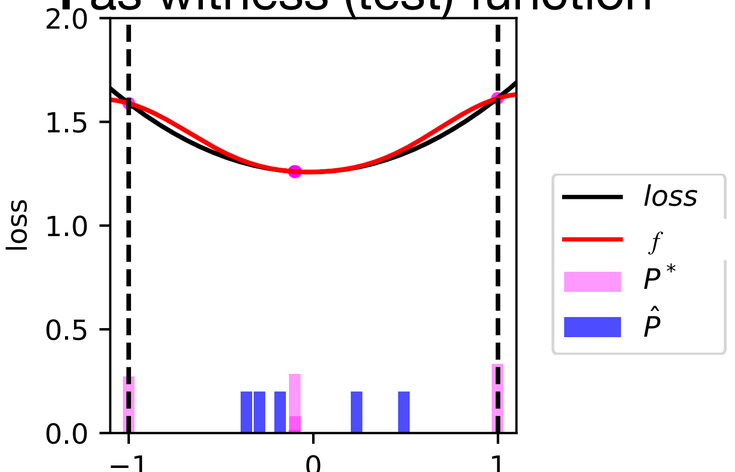

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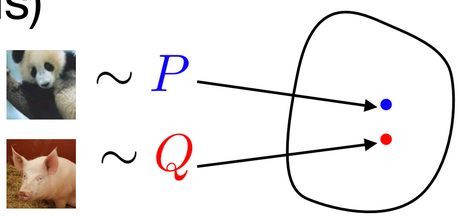


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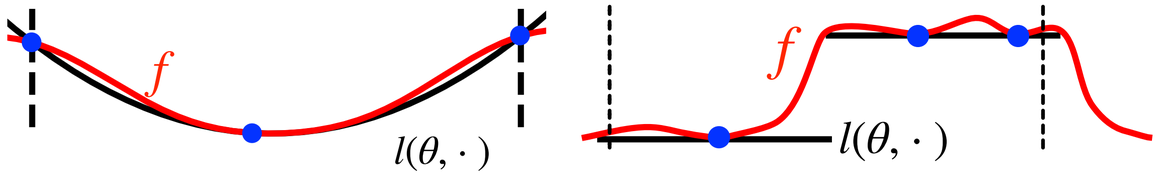


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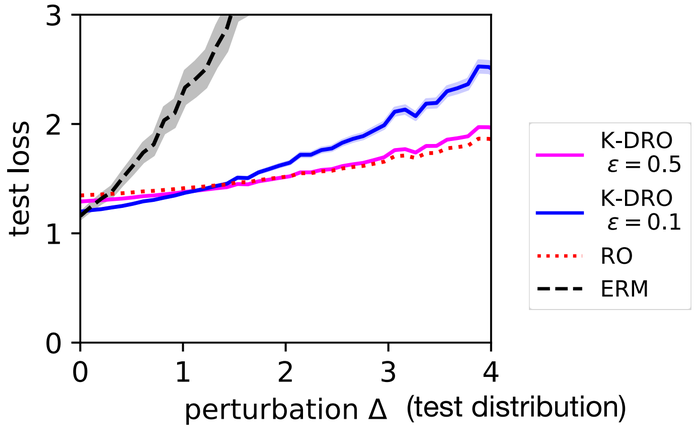


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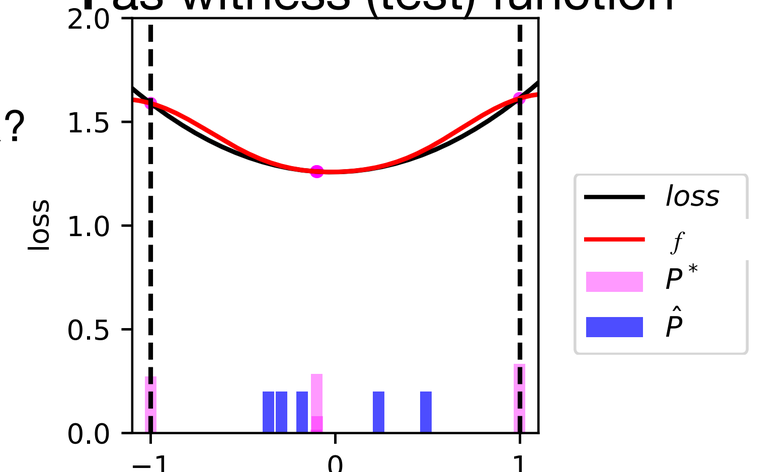

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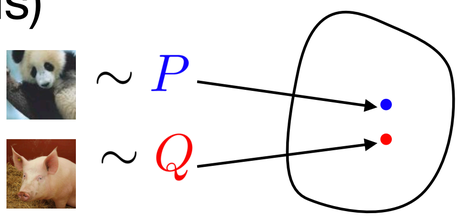


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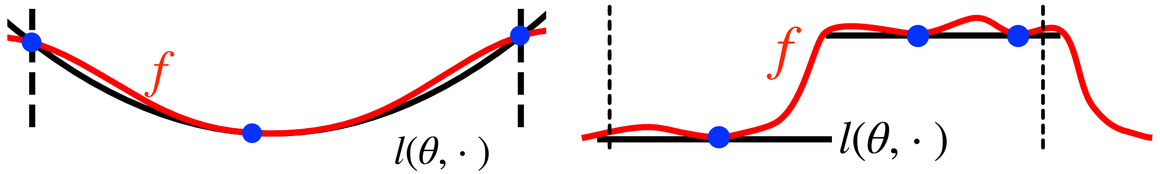


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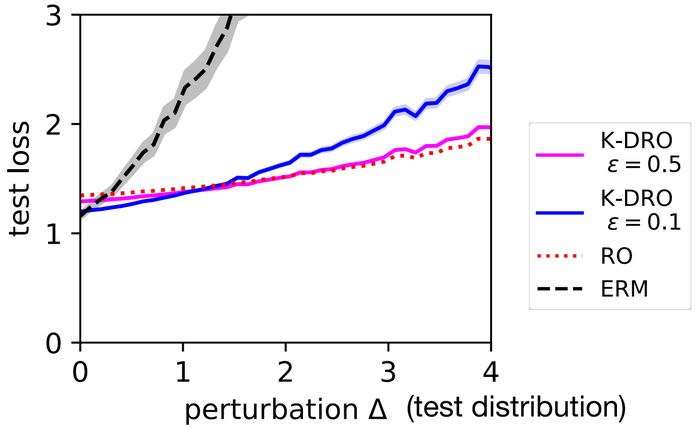


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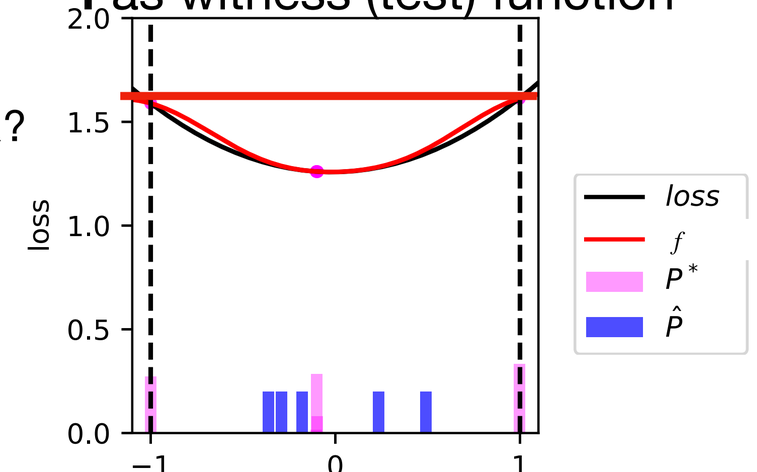

# Duality perspective

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2-Wasserstein

Primal: $\min_{\theta} \sup_{W_2(P,\hat{P})\leq\epsilon} \mathbb{E}_P\, l(\theta, \xi)$

Kernel DRO [**Z.** et al. 2021]

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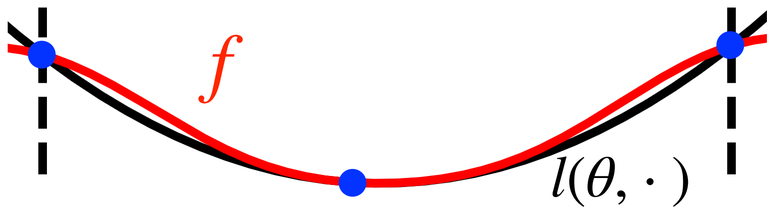

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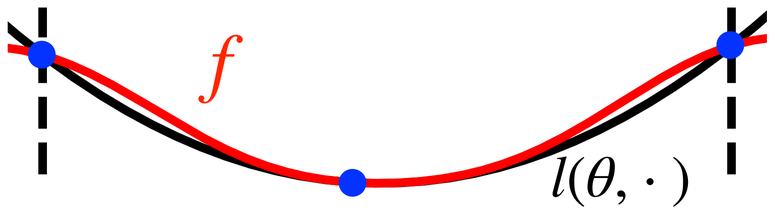

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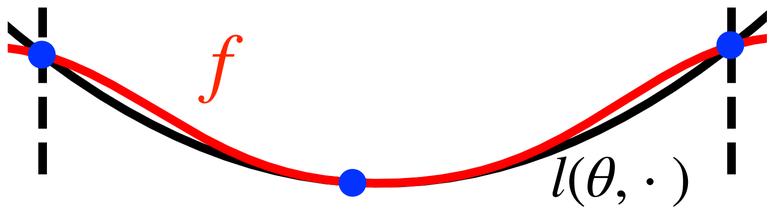

# Duality perspective

2-Wasserstein

Primal: $\min_{\theta} \sup_{W_2(P,\hat{P})\leq\epsilon} \mathbb{E}_P\, l(\theta,\xi)$

Dual: $\min_{\theta,\lambda>0} \frac{1}{N}\sum_{i=1}^{N} l_\theta^{\lambda\|\cdot\|^2}(\xi_i) + \lambda\epsilon^2$

where Moreau envelope

$l_\theta^{\lambda\|\cdot\|^2}(x) := \sup_u l(\theta,u) - \lambda\|u-x\|^2$

Considerations from WGF theory

- $l$ is **nonlinear** (e.g., DNN)?
- Nonlinear (in measure) energies?

Kernel DRO [**Z.** et al. 2021]

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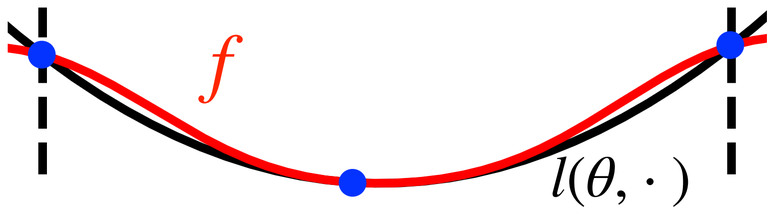


**Nonlinear** kernel approx. as robust surrogate losses (flatten the curve)

# Duality of
# Gradient Flow Force-Balance

# From static DRO to JKO scheme for gradient flows

DRO's Wasserstein measure optimization is not new.

$$\min_{\theta} \sup_{W_2(P,\hat{P})\leq\epsilon} \mathbb{E}_P\, l(\theta,\xi)$$

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**Wasserstein gradient flow** [Otto et al. 90s-2000s]. The Fokker-Planck equation

$$\partial_t \mu + \nabla \cdot (\mu \nabla \frac{\delta F}{\delta \mu}[\mu]) = 0$$

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**Jordan-Kinderlehrer-Otto (JKO) scheme** or Minimizing Movement Scheme (MMS):

$$\mu^{k+1} \in \inf_{\mu\in\mathcal{P}} F(\mu) + \frac{1}{2\tau} W_2^2(\mu,\mu^k)$$

generalizes the DRO dual reformulation of DRO to **nonlinear-in-measure** $F$.

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**Energy dissipation balance** (equality) via **Fenchel(-Young) duality and optimality**

$$\frac{\mathrm{d}}{\mathrm{d}t} f(x(t)) = {}_{X^*}\langle \nabla f(x(t)), \dot{x} \rangle_X = -\|\nabla f(x(t))\|^2 = -(\frac{1}{2}\|\dot{x}\|^2 + \frac{1}{2}\|\nabla f(x)\|^2)$$

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Energy does not necessarily decrease along non-solutions, i.e., only inequality

$$\langle \nabla f(z(t)), \dot{z} \rangle_X \geq -(\frac{1}{2}\|\dot{z}\|^2 + \frac{1}{2}\|\nabla f(z(t))\|^2).$$

# Duality in the Wasserstein gradient flow

In $(\mathrm{Prob}(\bar{X}), F, W_2)$, **Fenchel(-Young) duality** yields the **Energy dissipation balance** (equality) [Ambrosio et al. 2007]

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However, for some **nonlinear (in measure) energy** (e.g., in variational inference)

$$F(\mu) = \mathrm{D}_{\mathrm{KL}}(\mu \| \pi), \frac{\delta F}{\delta \mu}[\mu] = \log \rho - \log \pi,$$

the density $\rho := \frac{\mathrm{d}\mu}{\mathrm{d}\mathcal{L}}$ and hence the force field $\frac{\delta F}{\delta \mu}[\mu]$ are **not accessible** for atomic distributions $\mu$.

# Kernel gradient flow as dual space force-balance

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**Proposition**(informal). The gradient flow equation for $(\mathcal{P}(\bar{X}), F, \mathrm{MMD})$ is given by the **dual space (force-balance) kernel gradient flow**

$$k * \dot{\mu} = -g, \quad \text{where } \nabla g = \nabla \frac{\delta F}{\delta \mu}[\mu] \quad \mu\text{-a.e.}$$

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Compared with the Wasserstein GF of entropy, our kernel scheme approximates the (unavailable) "score function" $\nabla g = \nabla \log \rho$ in a principled geometry. This gives the interpretation of the dual kernel function in dynamics

$g$ **is the approximate (thermodynamic) force field.**

# Back to (kernel) robust learning

Motivated by our insight so far, in "Kernel DRO" [Zhu et al. 2021]

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On-going work: a **general-purpose measure optimization algorithm** motivated by this (see also the preprint on kernel mirror prox. [Dvurechensky & Zhu]).

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  - **optimal test fcn. for two-sample test**
  - **approx. force field**
- Other important uses of the dual kernel function: Causal inference, IV, conditional moments, (Robust) control and RL

This talk is based on previous and on-going joint works with many co-authors. Special thanks to Alexander Mielke for insightful discussions.

**Z.**, Jitkrittum, W., Diehl, M. & Schölkopf, B. Kernel Distributionally Robust Optimization. AISTATS 2021

Kremer, H., Nemmour, Y. , Schölkopf, B. & **Z.** Estimation Beyond Data Reweighting: Kernel Method of Moments. ICML 2023

P. Dvurechensky, **Z.**, Kernel Mirror Prox and RKHS Gradient Flow for Mixed Functional Nash Equilibrium. WIAS Preprint

**Z.**, Unbalanced Kernel Transport Problem. Working paper

Download the slides:

Website: jj-zhu.github.io