Duality from Distributionally Robust Learning to Gradient Flow Force-Balance

Jia-Jie Zhu
Weierstrass Institute for Applied Analysis and Stochastics
Berlin, Germany

DP4ML Workshop, International Conference on Machine Learning (ICML)
Honolulu Hawaii, USA, July 29th, 2023,

Weierstraß-Institut für
Angewandte Analysis und Stochastik

Duality of
Distributionally Robust Learning

Distributional **robustness**, but what kind?

Distributional robustness, but what kind?

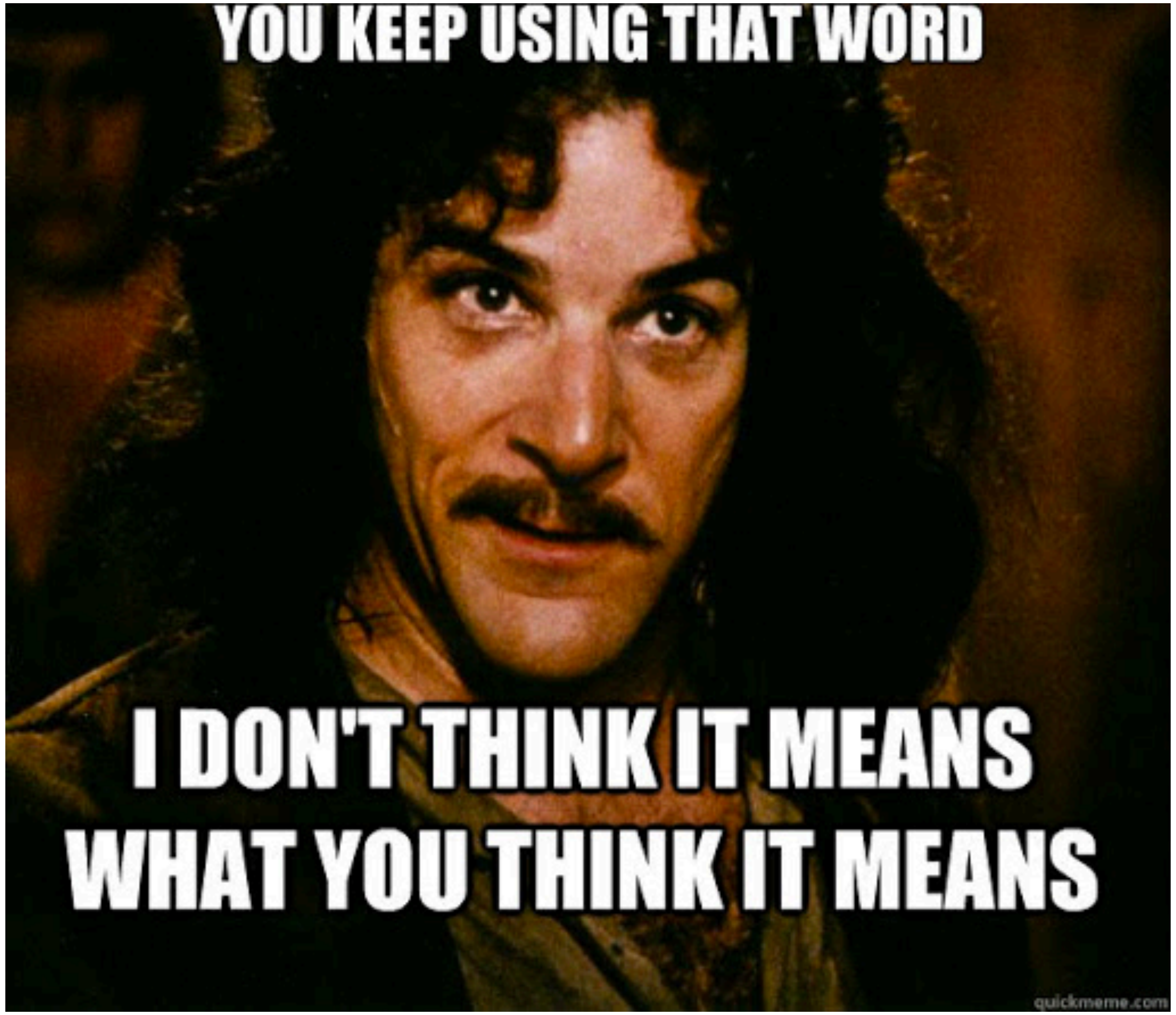


Figure credit: The Princess Bride,
a bedside story by your grandpa

From Statistical Learning to Distributionally Robust Learning

From Statistical Learning to Distributionally Robust Learning

Empirical Risk Minimization

$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} l(\theta, \xi_i), \quad \xi_i \sim P_0$$

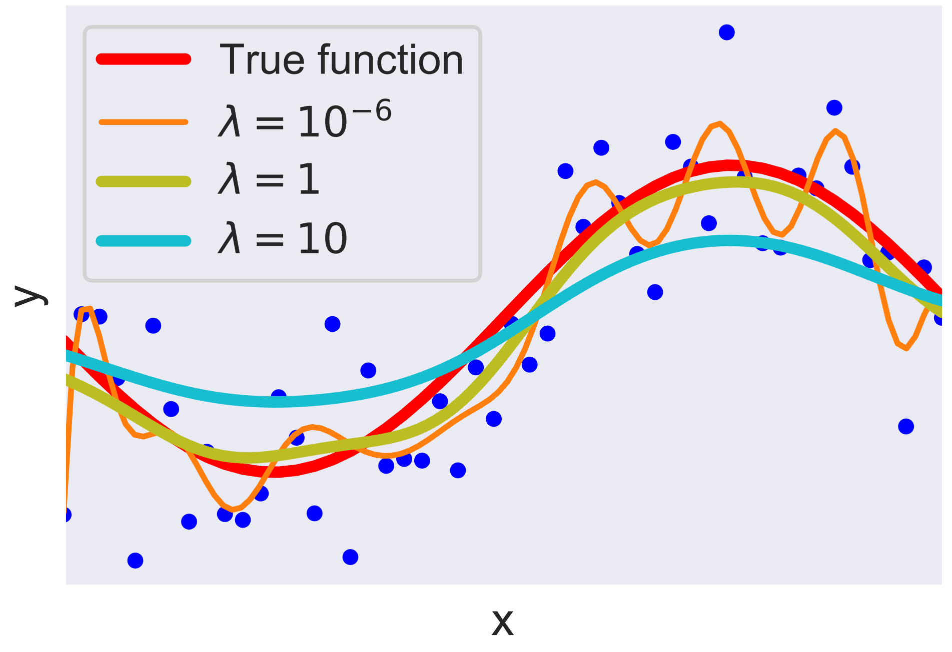
From Statistical Learning to Distributionally Robust Learning

Empirical Risk Minimization

$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} l(\theta, \xi_i), \quad \xi_i \sim P_0$$

- "Robust" under statistical fluctuation

$$\mathbb{E}_{P_0} l(\hat{\theta}, \xi) \leq \frac{1}{N} \sum_{i=1}^{N} l(\hat{\theta}, \xi_i) + \mathcal{O}(\frac{1}{\sqrt{N}})$$



From Statistical Learning to Distributionally Robust Learning

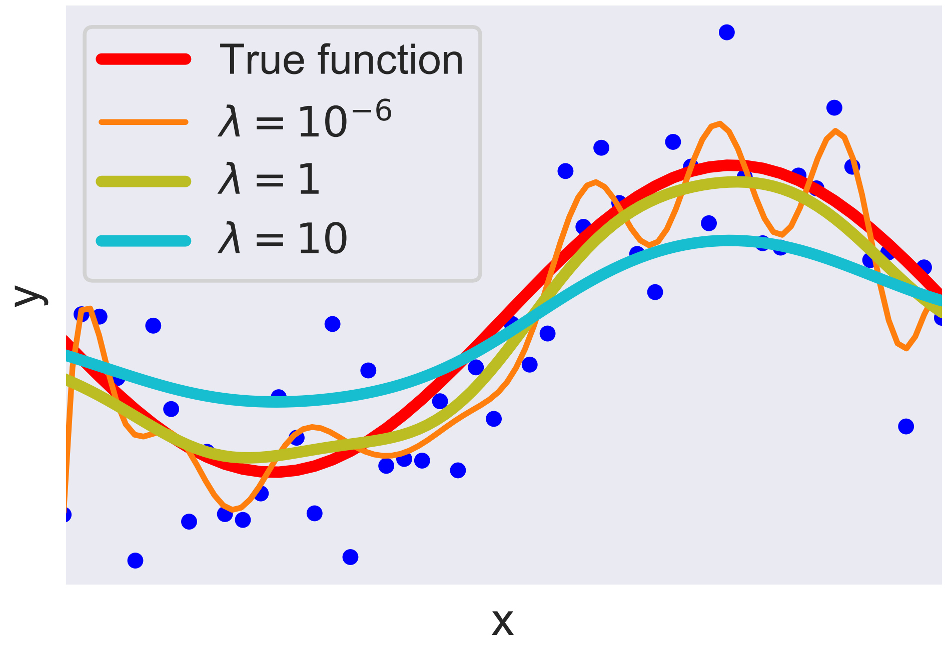
Empirical Risk Minimization

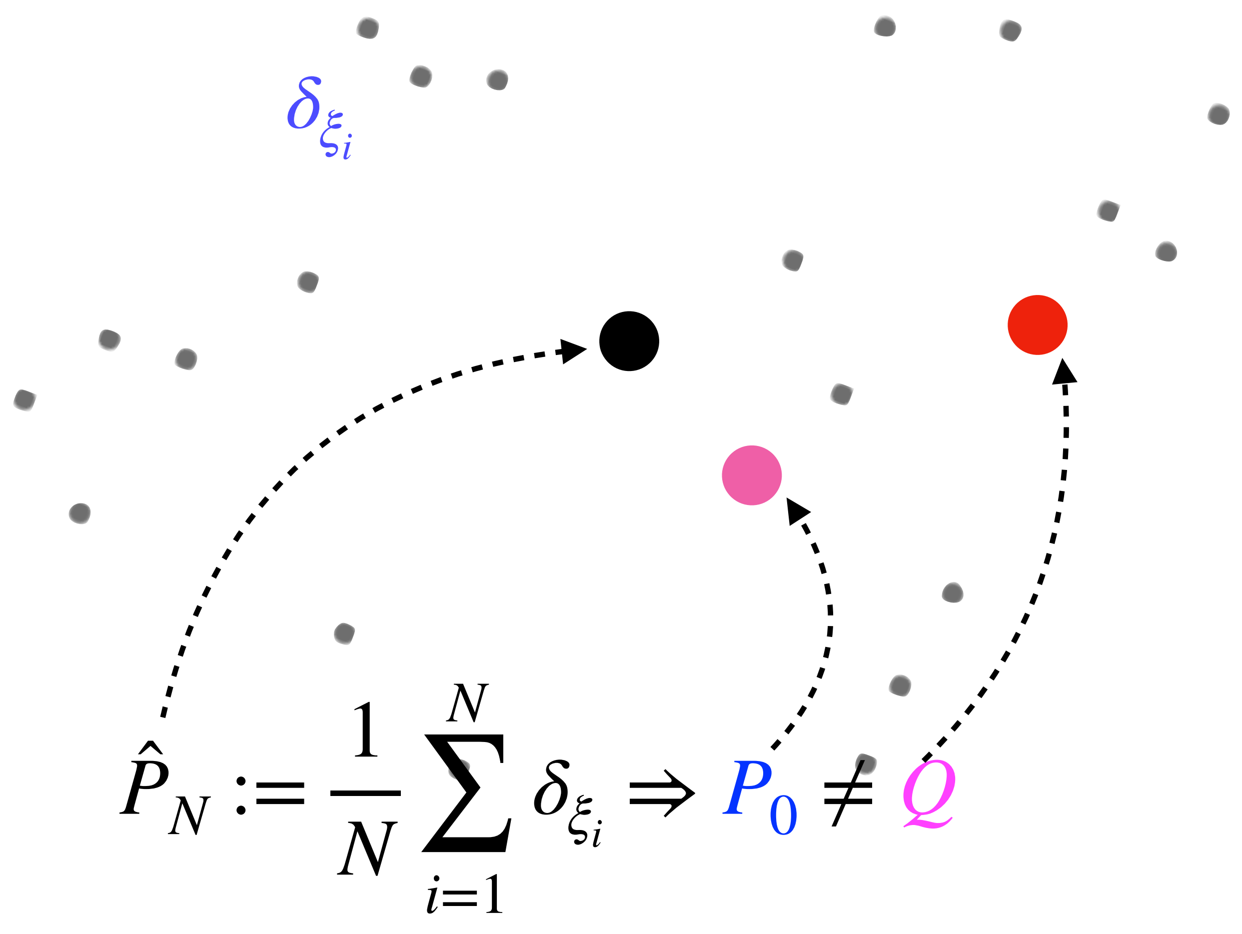
$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} l(\theta, \xi_i), \quad \xi_i \sim P_0$$

- "Robust" under statistical fluctuation

$$\mathbb{E}_{P_0} l(\hat{\theta}, \xi) \leq \frac{1}{N} \sum_{i=1}^{N} l(\hat{\theta}, \xi_i) + \mathcal{O}(\frac{1}{\sqrt{N}})$$

- Not robust under data distribution shifts, when Q $(\neq P_0)$





From Statistical Learning to Distributionally Robust Learning

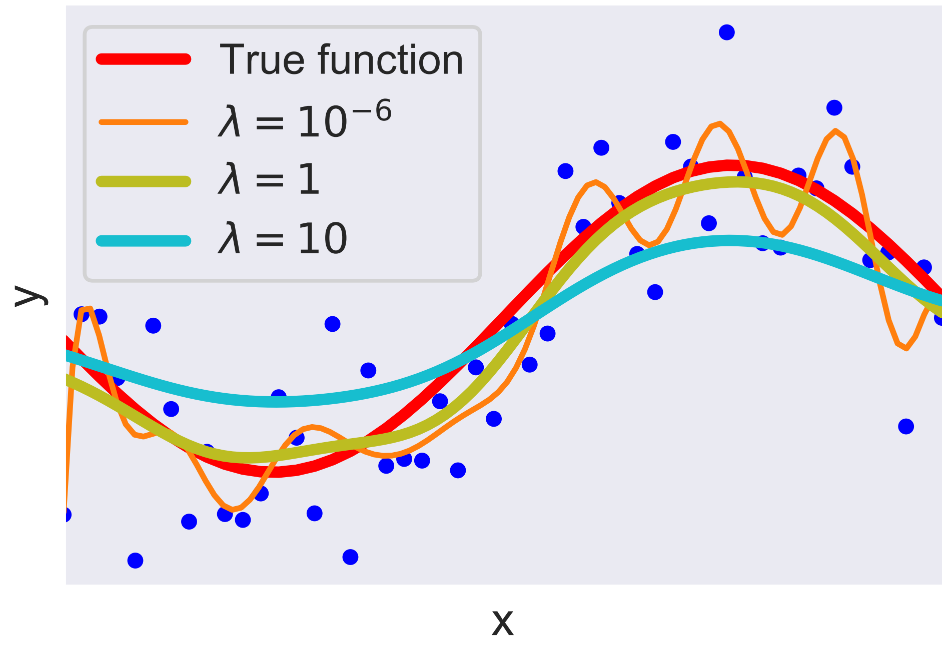
Empirical Risk Minimization

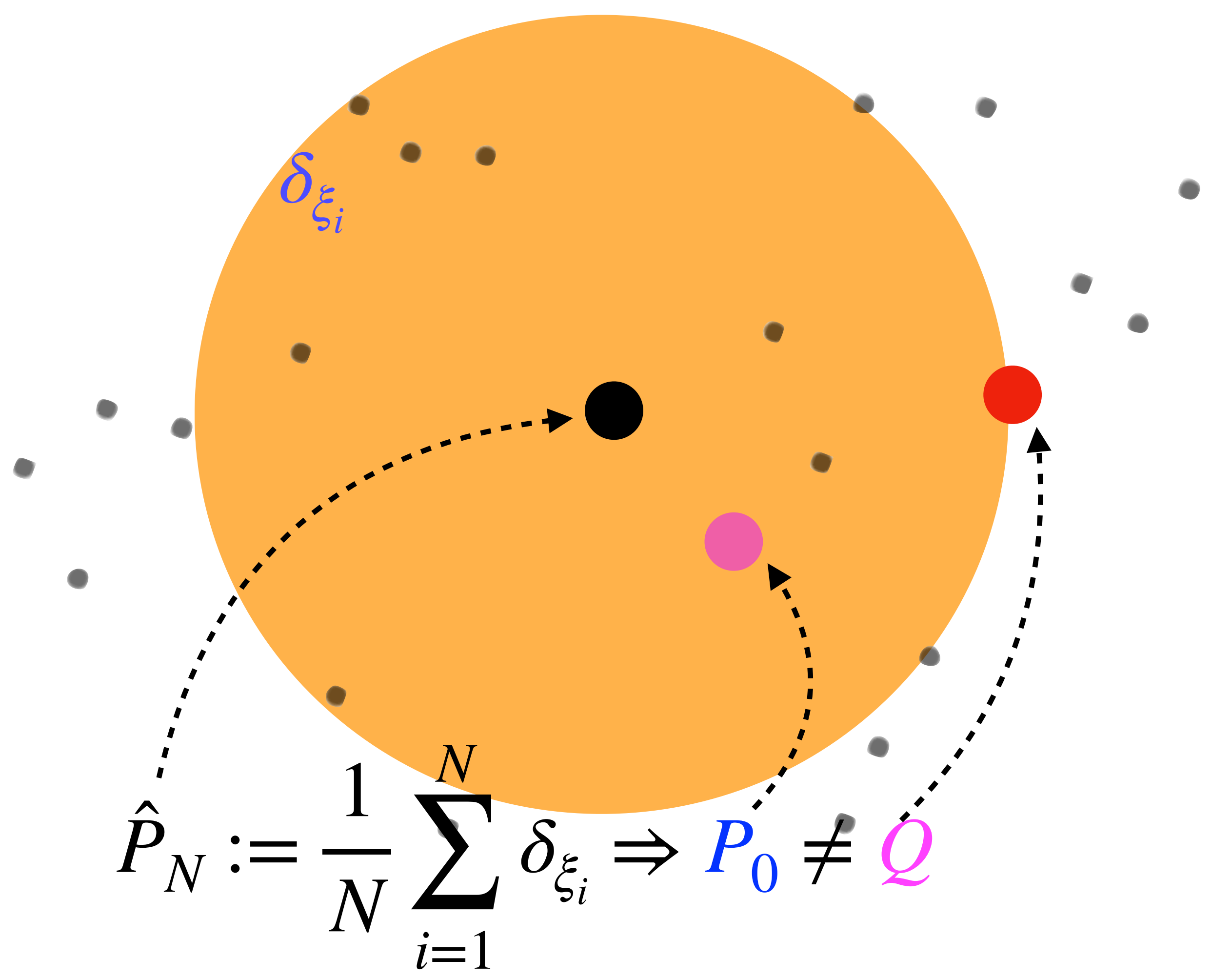
$$\min_{\theta} \frac{1}{N}\sum_{i=1}^{N} l(\theta, \xi_i), \quad \xi_i \sim P_0$$

- "Robust" under statistical fluctuation

$$\mathbb{E}_{P_0} l(\hat{\theta}, \xi) \leq \frac{1}{N}\sum_{i=1}^{N} l(\hat{\theta}, \xi_i) + \mathcal{O}(\frac{1}{\sqrt{N}})$$

- Not robust under data distribution shifts, when $Q \ (\neq P_0)$





Distributionally Robust Optimization (DRO)

$$\min_{\theta} \sup_{Q \in \mathcal{M}} \mathbb{E}_Q l(\theta, \xi)$$

From Statistical Learning to Distributionally Robust Learning

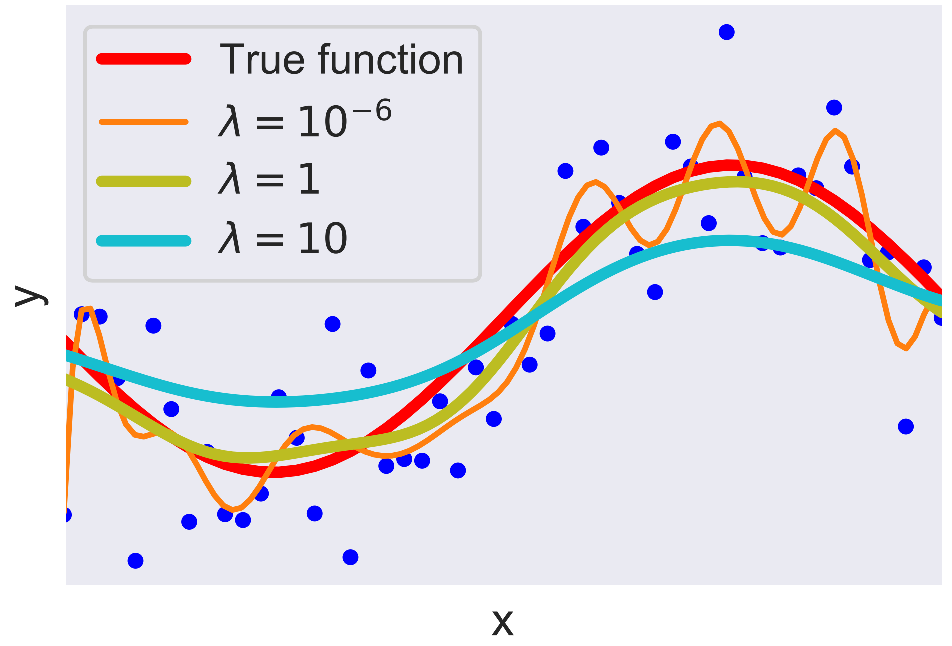
Empirical Risk Minimization

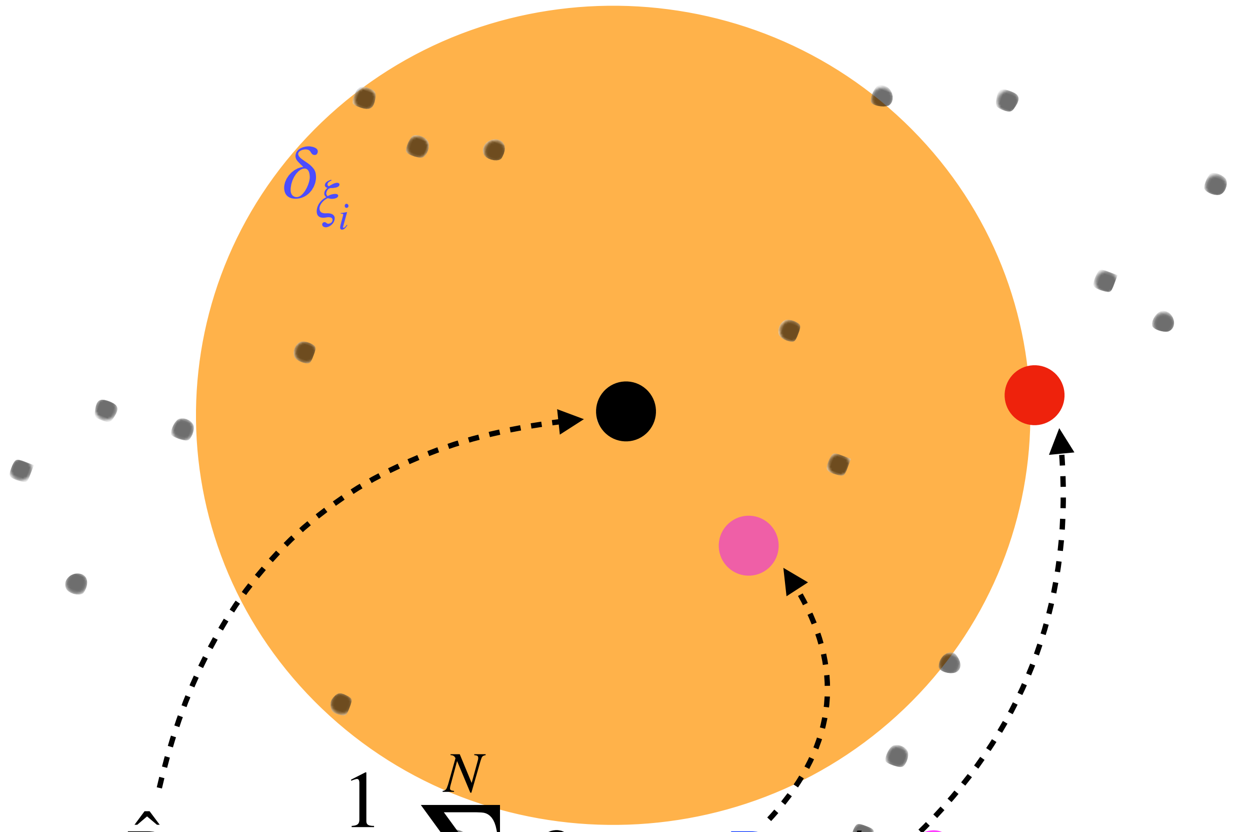
$$\min_{\theta} \frac{1}{N}\sum_{i=1}^{N} l(\theta, \xi_i), \quad \xi_i \sim P_0$$

- "Robust" under statistical fluctuation

$$\mathbb{E}_{P_0} l(\hat{\theta}, \xi) \leq \frac{1}{N}\sum_{i=1}^{N} l(\hat{\theta}, \xi_i) + \mathcal{O}(\frac{1}{\sqrt{N}})$$

- Not robust under data distribution shifts, when Q $(\neq P_0)$





$$\hat{P}_N := \frac{1}{N}\sum_{i=1}^{N} \delta_{\xi_i} \Rightarrow P_0 \neq Q$$

Distributionally Robust Optimization (DRO)

$$\min_{\theta} \sup_{Q \in \mathcal{M}} \mathbb{E}_Q l(\theta, \xi)$$

Worst-case distribution Q within the ambiguity set $\mathcal{M}$ [Delage & Ye 2010] in certain geometry.

From Statistical Learning to Distributionally Robust Learning

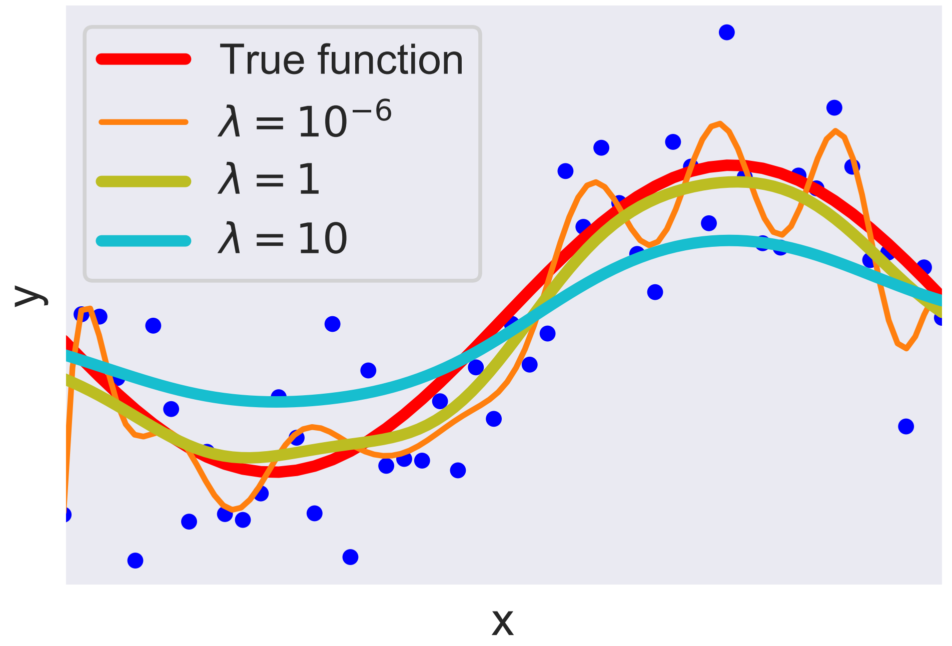
Empirical Risk Minimization

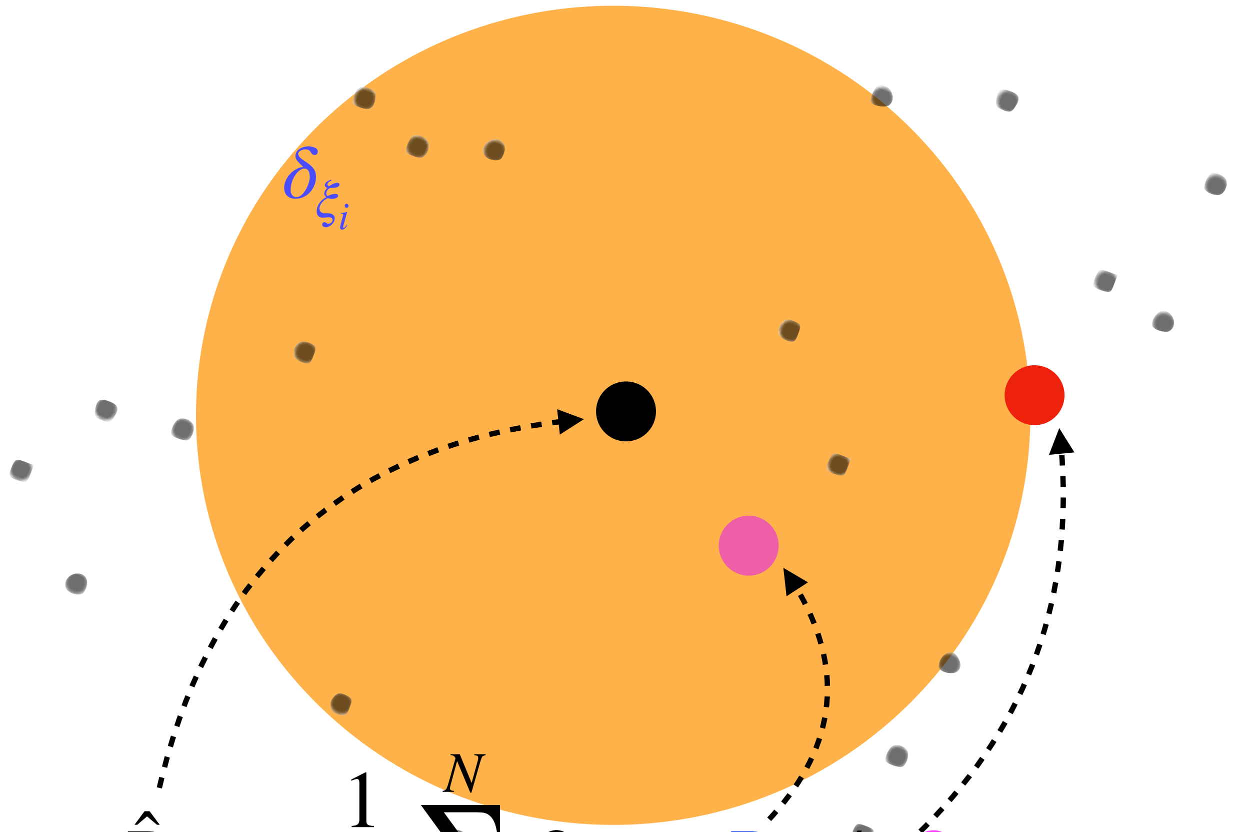
$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} l(\theta, \xi_i), \quad \xi_i \sim P_0$$

- "Robust" under statistical fluctuation

$$\mathbb{E}_{P_0} l(\hat{\theta}, \xi) \leq \frac{1}{N} \sum_{i=1}^{N} l(\hat{\theta}, \xi_i) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

- Not robust under data distribution shifts, when $Q \; (\neq P_0)$





$$\hat{P}_N := \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_i} \Rightarrow P_0 \neq Q$$

Distributionally Robust Optimization (DRO)

$$\min_{\theta} \sup_{Q \in \mathcal{M}} \mathbb{E}_Q l(\theta, \xi)$$

Worst-case distribution Q within the ambiguity set $\mathcal{M}$ [Delage & Ye 2010] in certain geometry.

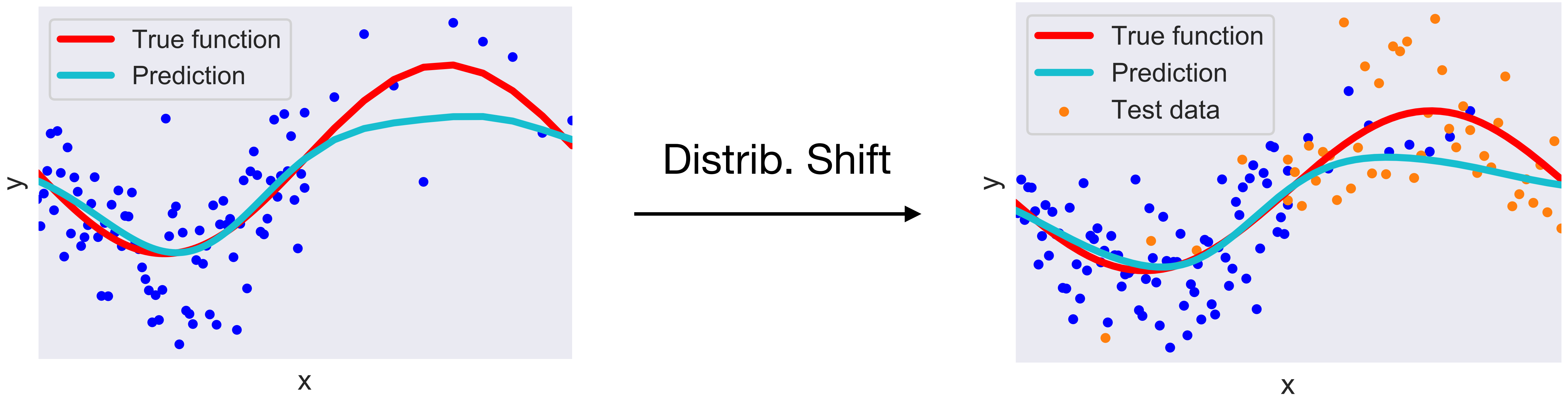


Figure credit: Heiner Kremer

From Statistical Learning to Distributionally Robust Learning

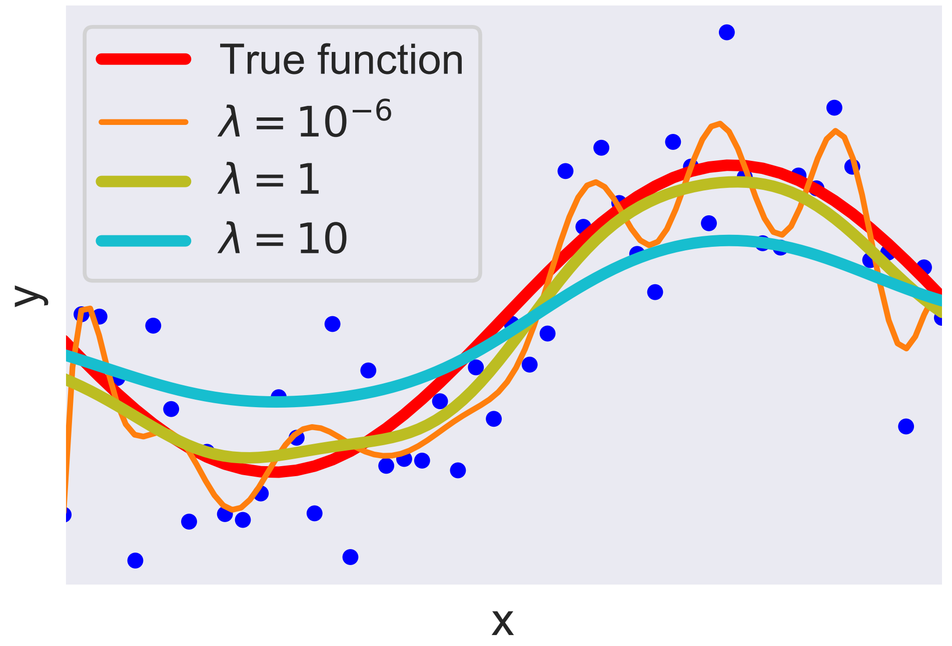
Empirical Risk Minimization

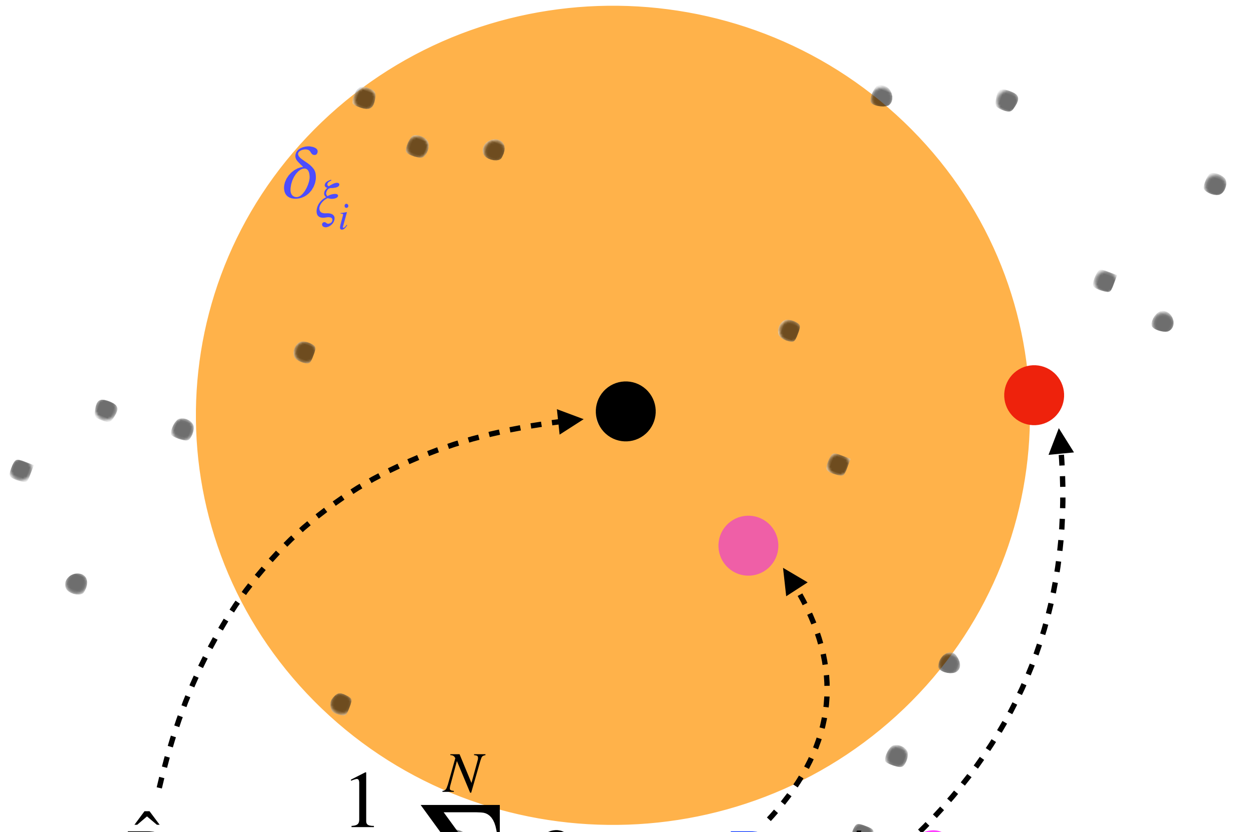
$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} l(\theta, \xi_i), \quad \xi_i \sim P_0$$

- "Robust" under statistical fluctuation

$$\mathbb{E}_{P_0} l(\hat{\theta}, \xi) \le \frac{1}{N} \sum_{i=1}^{N} l(\hat{\theta}, \xi_i) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

- Not robust under data distribution shifts, when Q $(\neq P_0)$



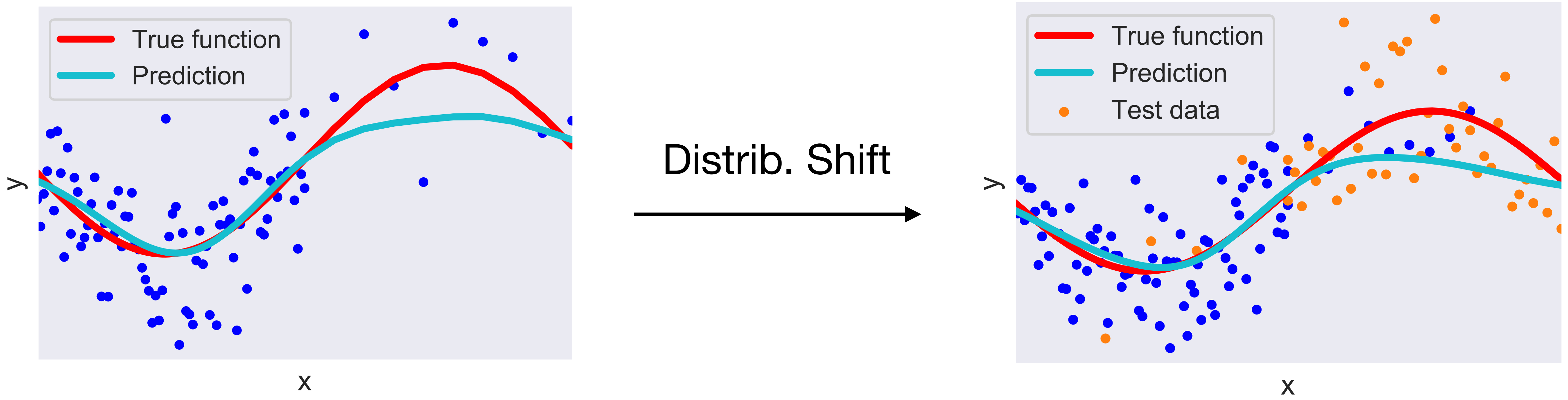


$$\hat{P}_N := \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_i} \Rightarrow P_0 \neq Q$$

Distributionally Robust Optimization (DRO)

$$\min_{\theta} \sup_{Q \in \mathcal{M}} \mathbb{E}_Q l(\theta, \xi)$$

Worst-case distribution Q within the ambiguity set $\mathcal{M}$ [Delage & Ye 2010] in certain geometry.



Why study new geometry?

Figure credit: Heiner Kremer

From Statistical Learning to Distributionally Robust Learning

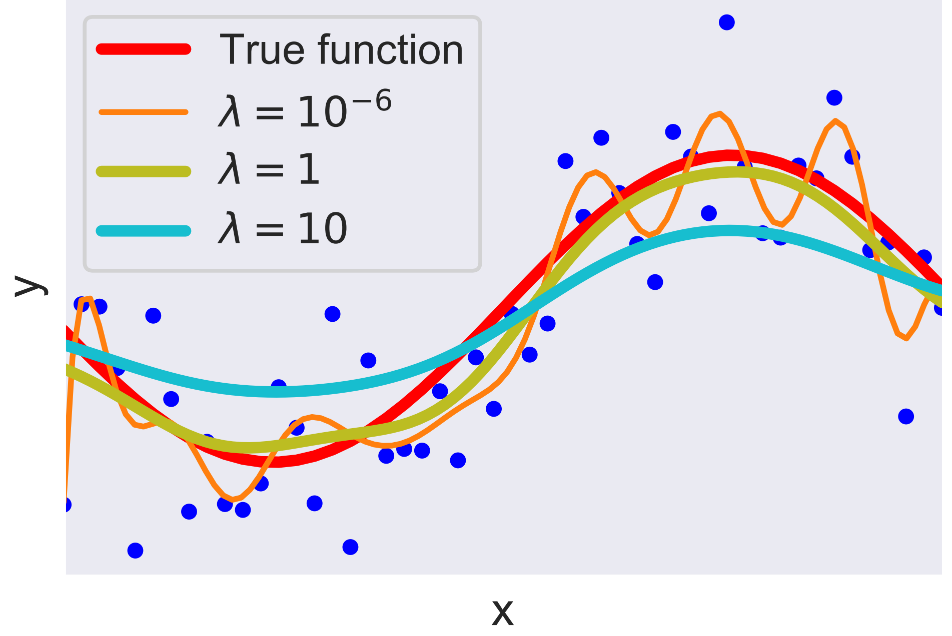
Empirical Risk Minimization

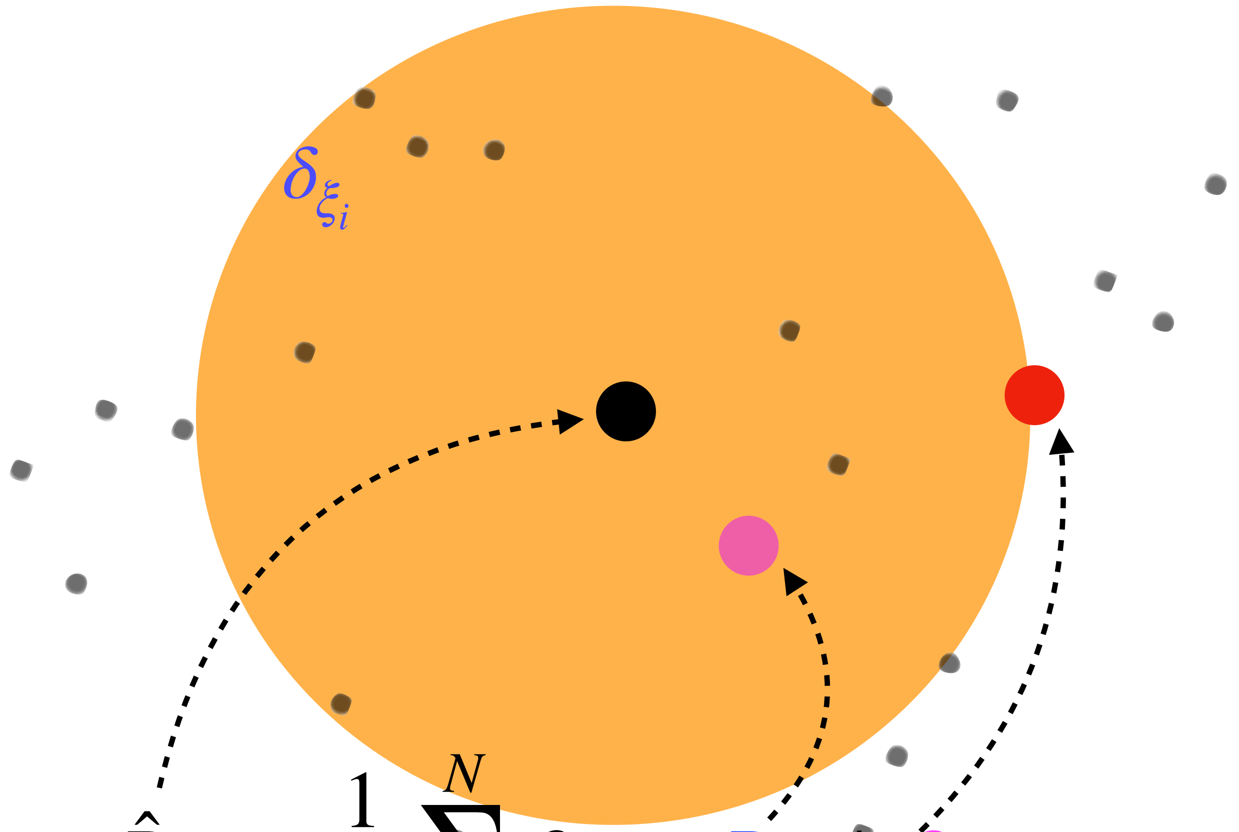
$$\min_\theta \frac{1}{N}\sum_{i=1}^{N} l(\theta,\xi_i), \quad \xi_i \sim P_0$$

- "Robust" under statistical fluctuation

$$\mathbb{E}_{P_0} l(\hat\theta,\xi) \le \frac{1}{N}\sum_{i=1}^{N} l(\hat\theta,\xi_i) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

- Not robust under data distribution shifts, when Q $(\neq P_0)$



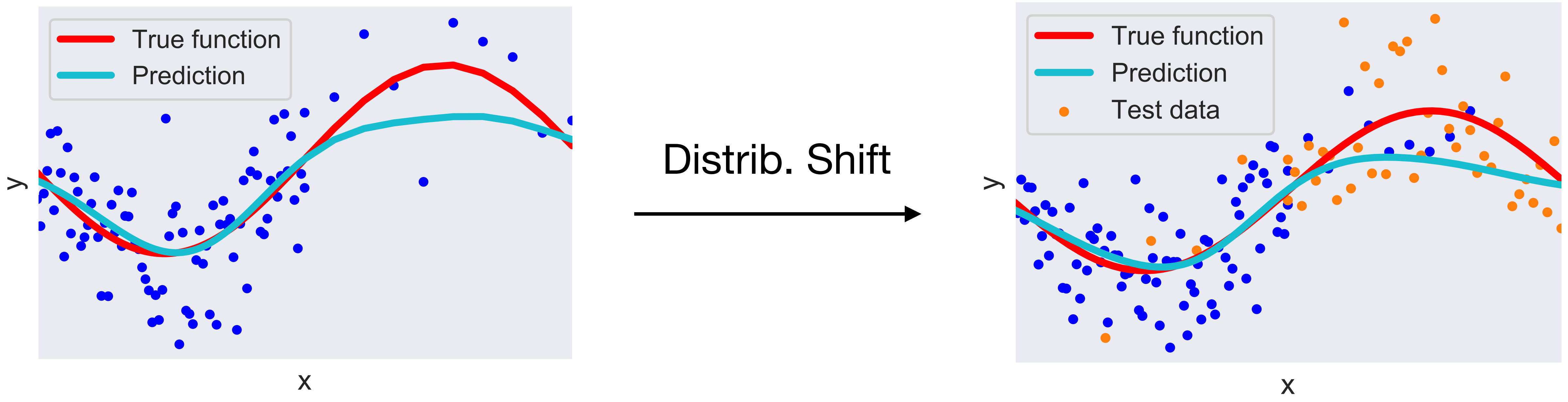


$$\hat P_N := \frac{1}{N}\sum_{i=1}^{N}\delta_{\xi_i} \Rightarrow P_0 \neq Q$$

Distributionally Robust Optimization (DRO)

$$\min_\theta \sup_{Q\in\mathcal{M}} \mathbb{E}_Q l(\theta,\xi)$$

Worst-case distribution Q within the ambiguity set $\mathcal{M}$ [Delage & Ye 2010] in certain geometry.



Why study new geometry?

New geometries leading to new fields of research and breakthroughs:

Figure credit: Heiner Kremer

From Statistical Learning to Distributionally Robust Learning

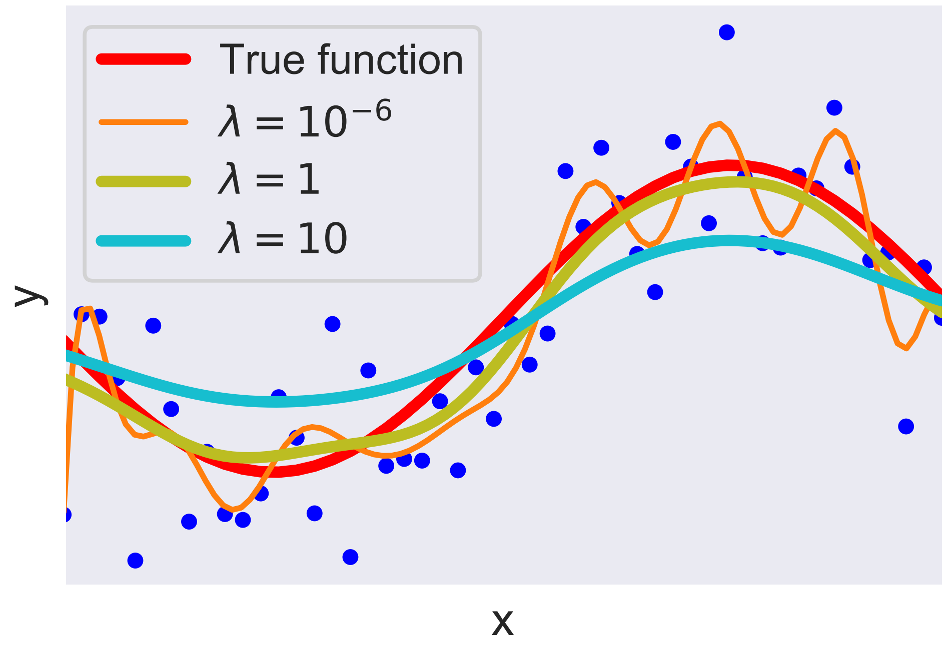
Empirical Risk Minimization

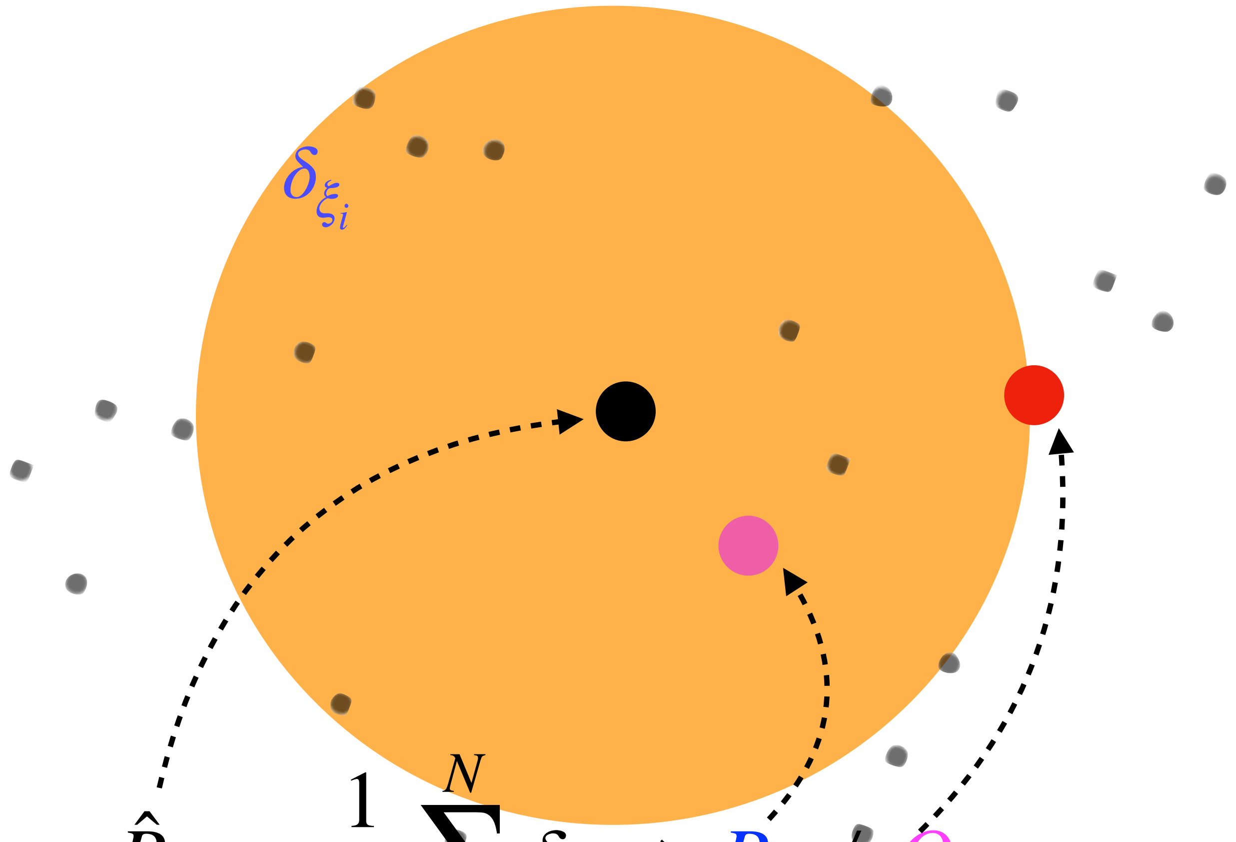
$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} l(\theta, \xi_i), \quad \xi_i \sim P_0$$

- "Robust" under statistical fluctuation

$$\mathbb{E}_{P_0} l(\hat{\theta}, \xi) \leq \frac{1}{N} \sum_{i=1}^{N} l(\hat{\theta}, \xi_i) + \mathcal{O}(\frac{1}{\sqrt{N}})$$

- Not robust under data distribution shifts, when Q $(\neq P_0)$



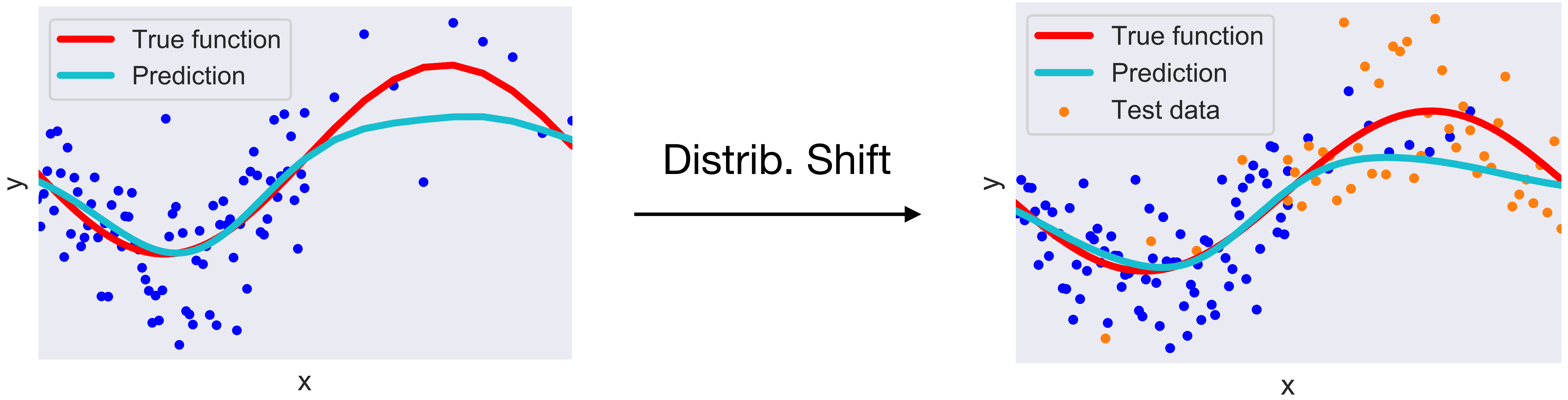


$$\hat{P}_N := \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_i} \Rightarrow P_0 \neq Q$$

Distributionally Robust Optimization (DRO)

$$\min_{\theta} \sup_{Q \in \mathcal{M}} \mathbb{E}_{Q} l(\theta, \xi)$$

Worst-case distribution Q within the ambiguity set $\mathcal{M}$ [Delage & Ye 2010] in certain geometry.



Why study new geometry?

New geometries leading to new fields of research and breakthroughs:

Information geometry [S. Amari et al.] e.g. natural gradient descent in Fisher-Rao geometry.

Figure credit: Heiner Kremer

From Statistical Learning to Distributionally Robust Learning

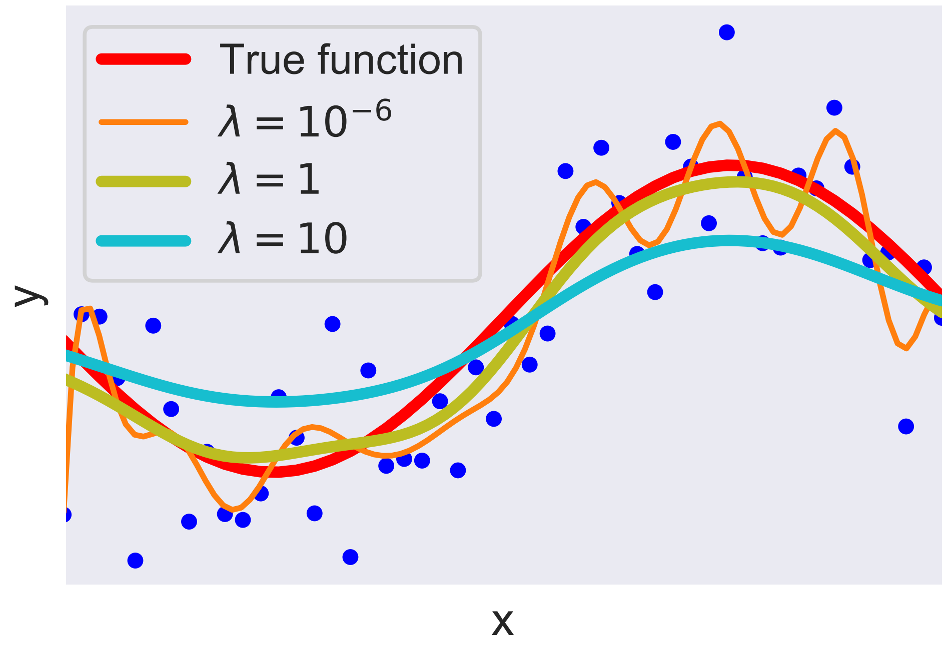
Empirical Risk Minimization

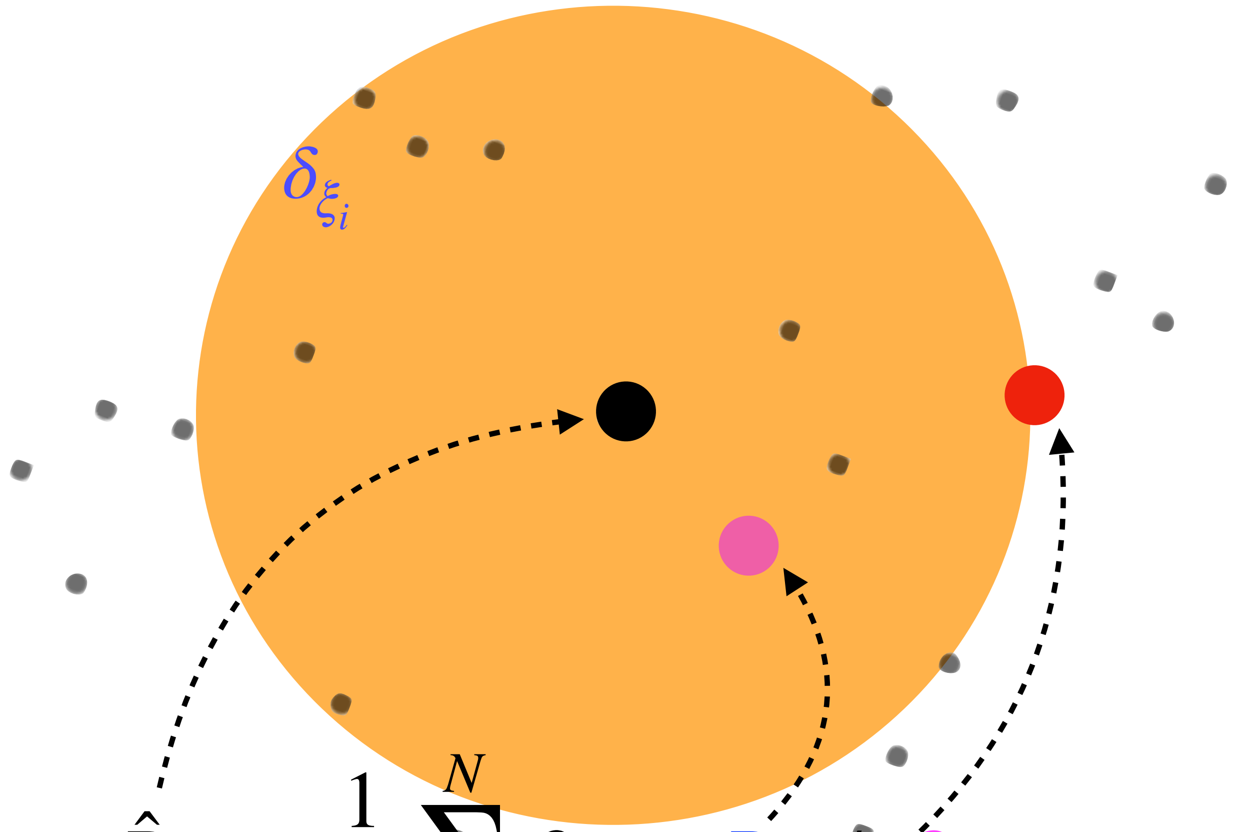
$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} l(\theta, \xi_i), \quad \xi_i \sim P_0$$

- "Robust" under statistical fluctuation

$$\mathbb{E}_{P_0} l(\hat{\theta}, \xi) \leq \frac{1}{N} \sum_{i=1}^{N} l(\hat{\theta}, \xi_i) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

- Not robust under data distribution shifts, when Q ($\neq P_0$)



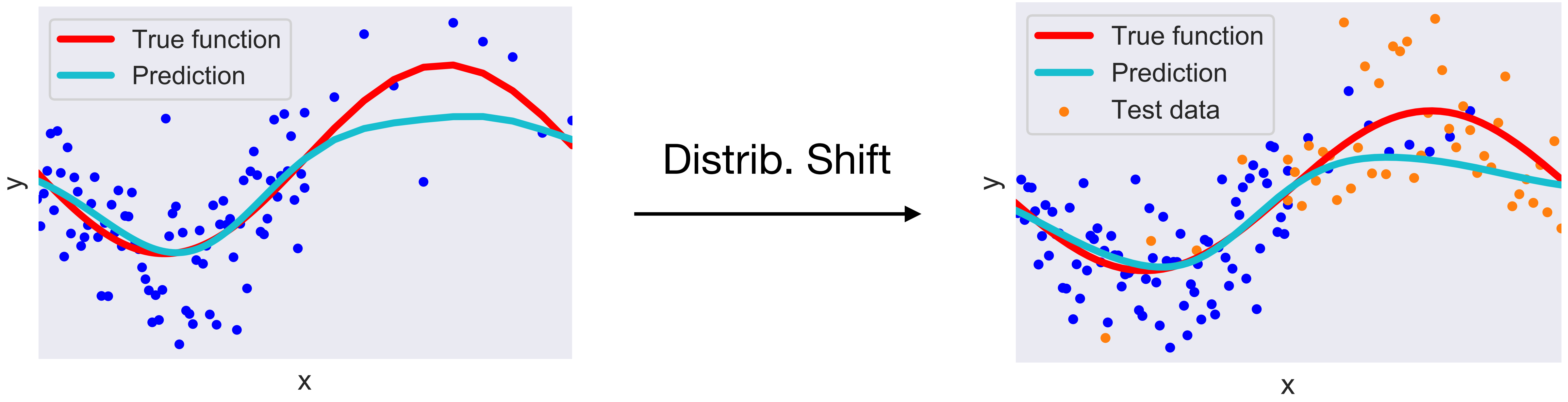


$$\hat{P}_N := \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_i} \Rightarrow P_0 \neq Q$$

Distributionally Robust Optimization (DRO)

$$\min_{\theta} \sup_{Q \in \mathcal{M}} \mathbb{E}_Q l(\theta, \xi)$$

Worst-case distribution Q within the ambiguity set $\mathcal{M}$ [Delage & Ye 2010] in certain geometry.



Why study new geometry?

New geometries leading to new fields of research and breakthroughs:

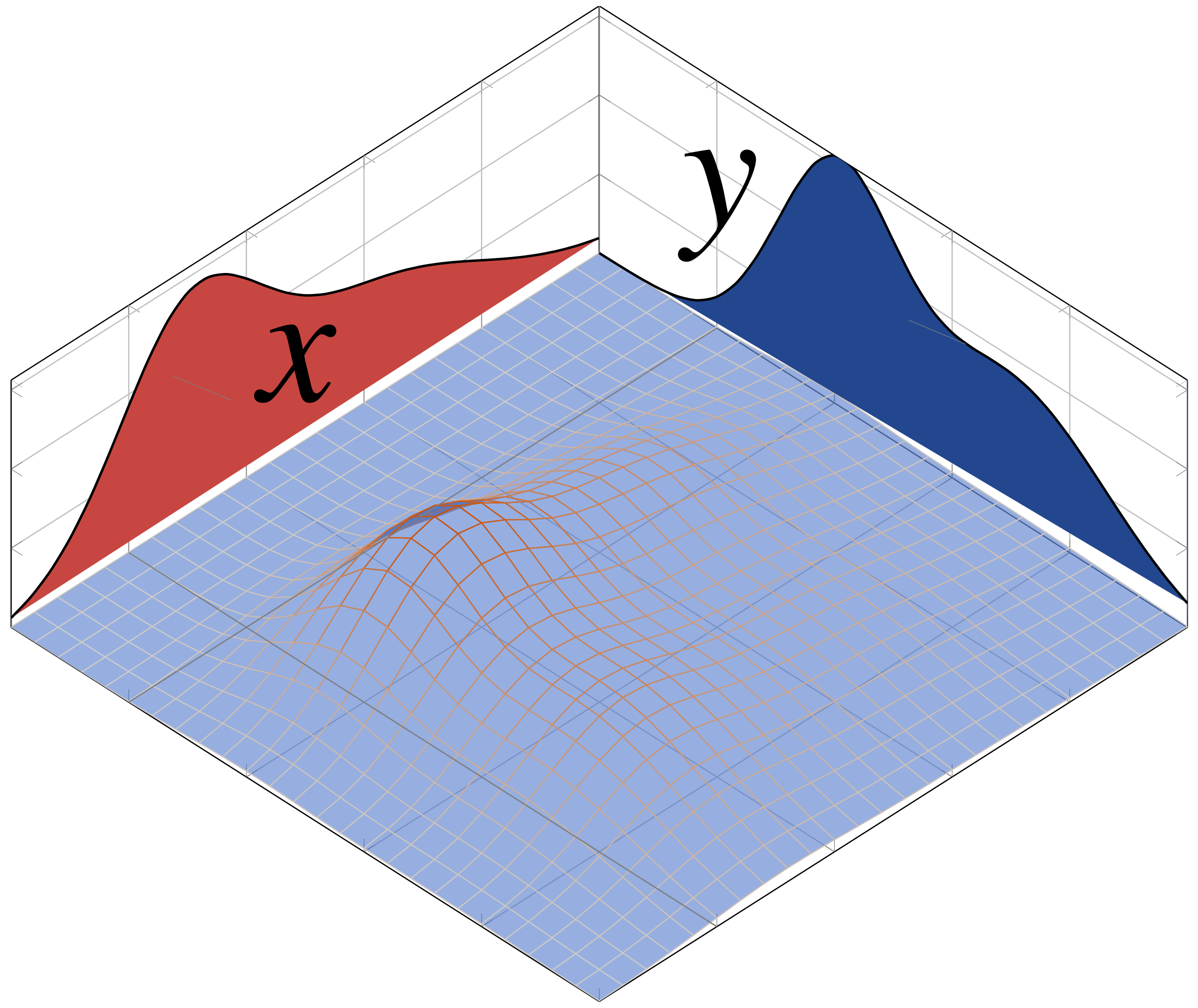
Information geometry [S. Amari et al.] e.g. natural gradient descent in Fisher-Rao geometry.

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

Figure credit: Heiner Kremer

Background: Wasserstein Geometry

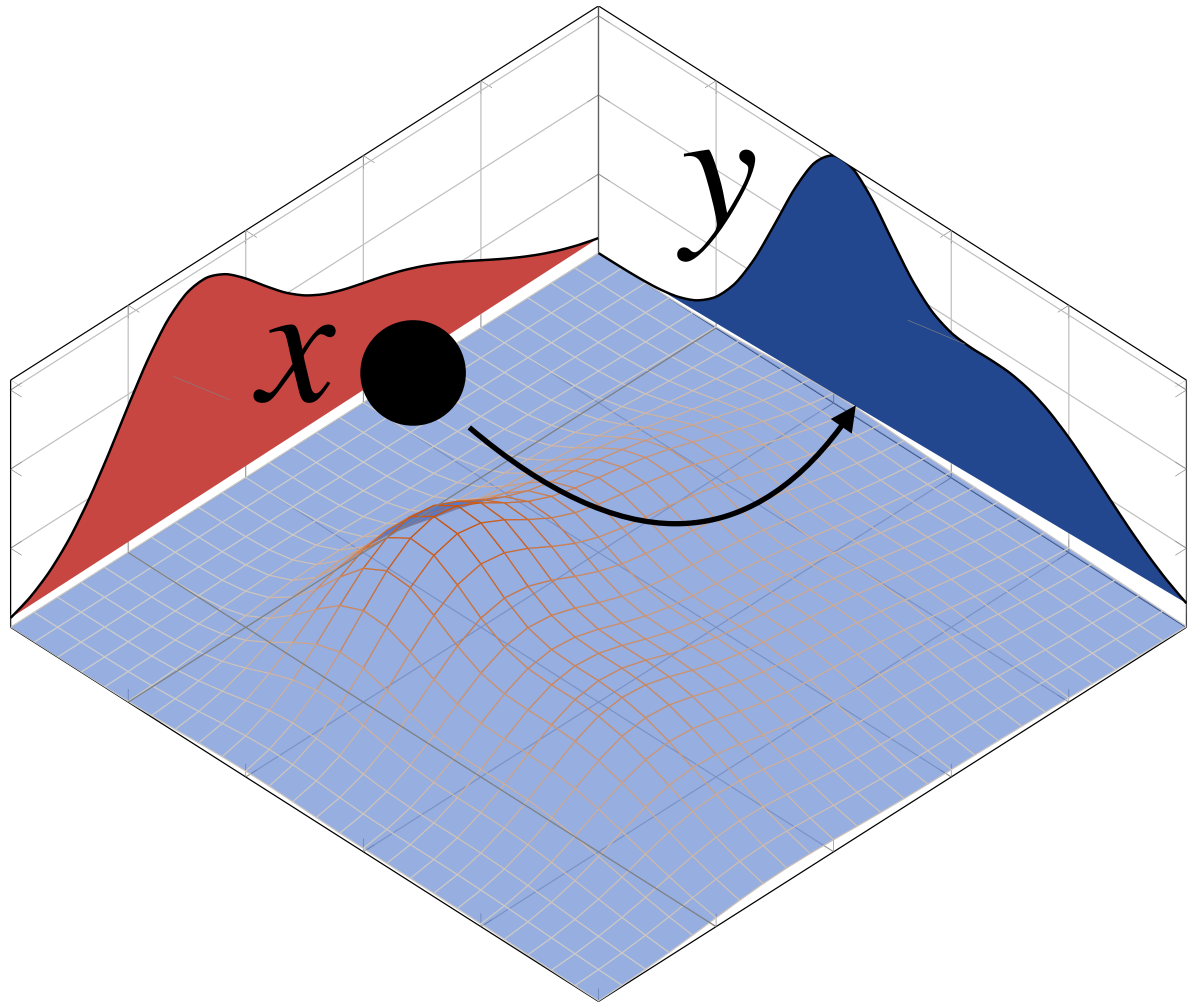
Background: Wasserstein Geometry



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

$$W_p^p(P, Q) := \inf \left\{ \int |x - y|^p \, d\Pi(x, y) \,\middle|\, \pi_\#^{(1)}\Pi = P,\ \pi_\#^{(2)}\Pi = Q \right\}$$

Background: Wasserstein Geometry



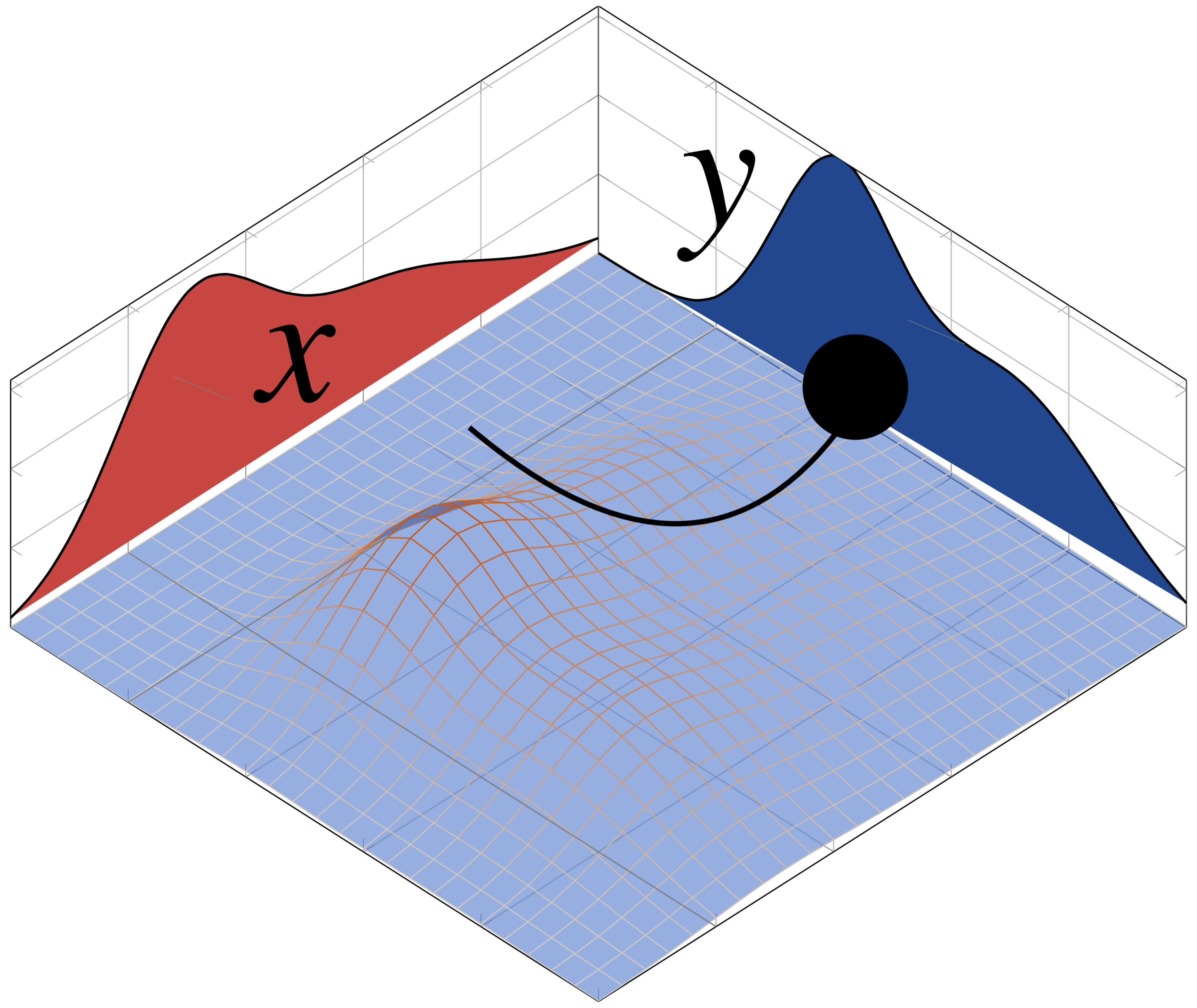
Definition. The p-**Wasserstein distance** between probability measures P, Q on $\mathbb{R}^d$ (with p finite moments, $p \geq 1$) is defined through the following Kantorovich problem

$$W_p^p(P, Q) := \inf \left\{ \int |x - y|^p \, d\Pi(x, y) \,\middle|\, \pi_\#^{(1)}\Pi = P,\ \pi_\#^{(2)}\Pi = Q \right\}$$

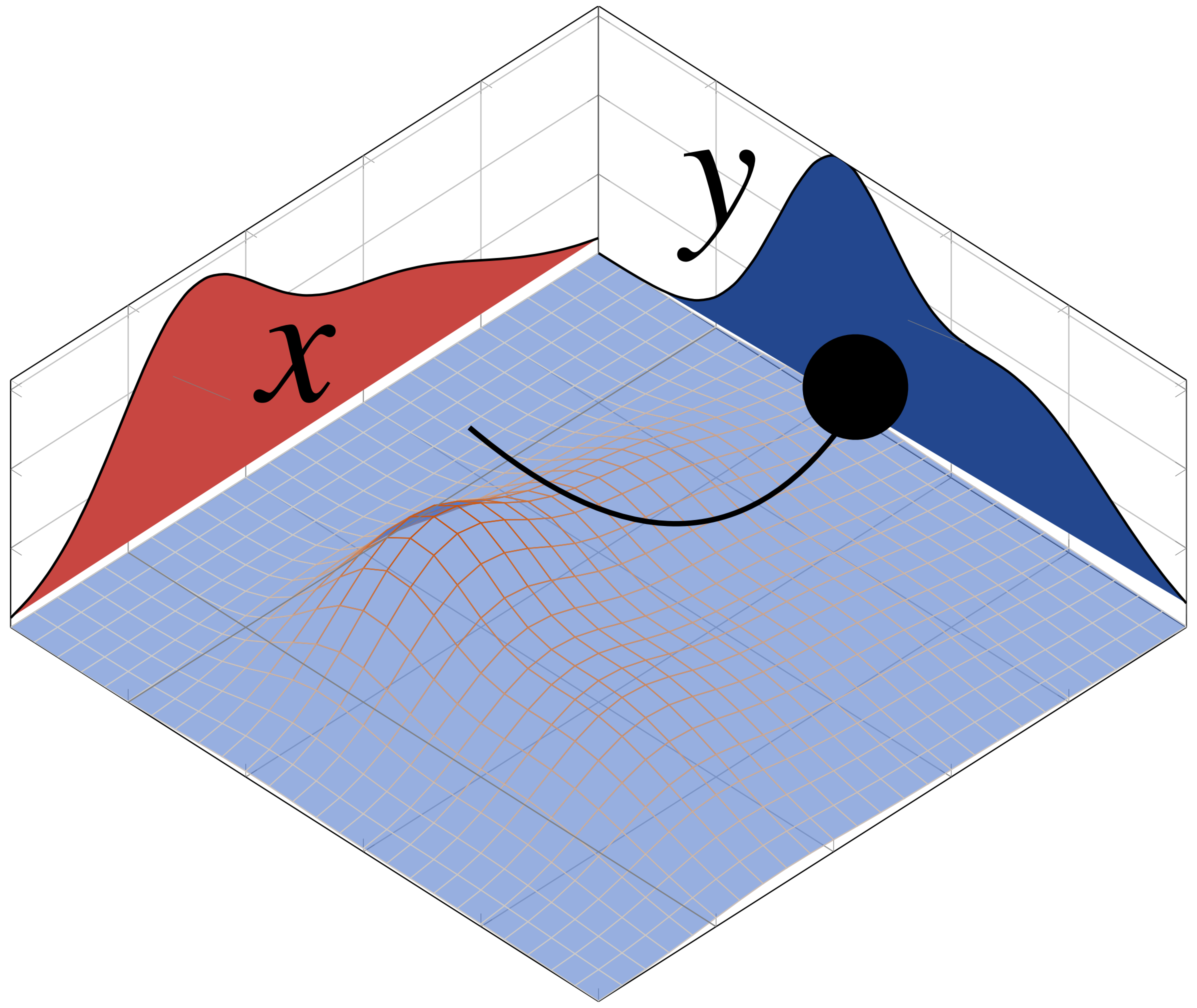
Background: Wasserstein Geometry

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

$$W_p^p(P, Q) := \inf \left\{ \int |x - y|^p \, d\Pi(x, y) \,\middle|\, \pi_\#^{(1)}\Pi = P, \; \pi_\#^{(2)}\Pi = Q \right\}$$



Background: Wasserstein Geometry



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

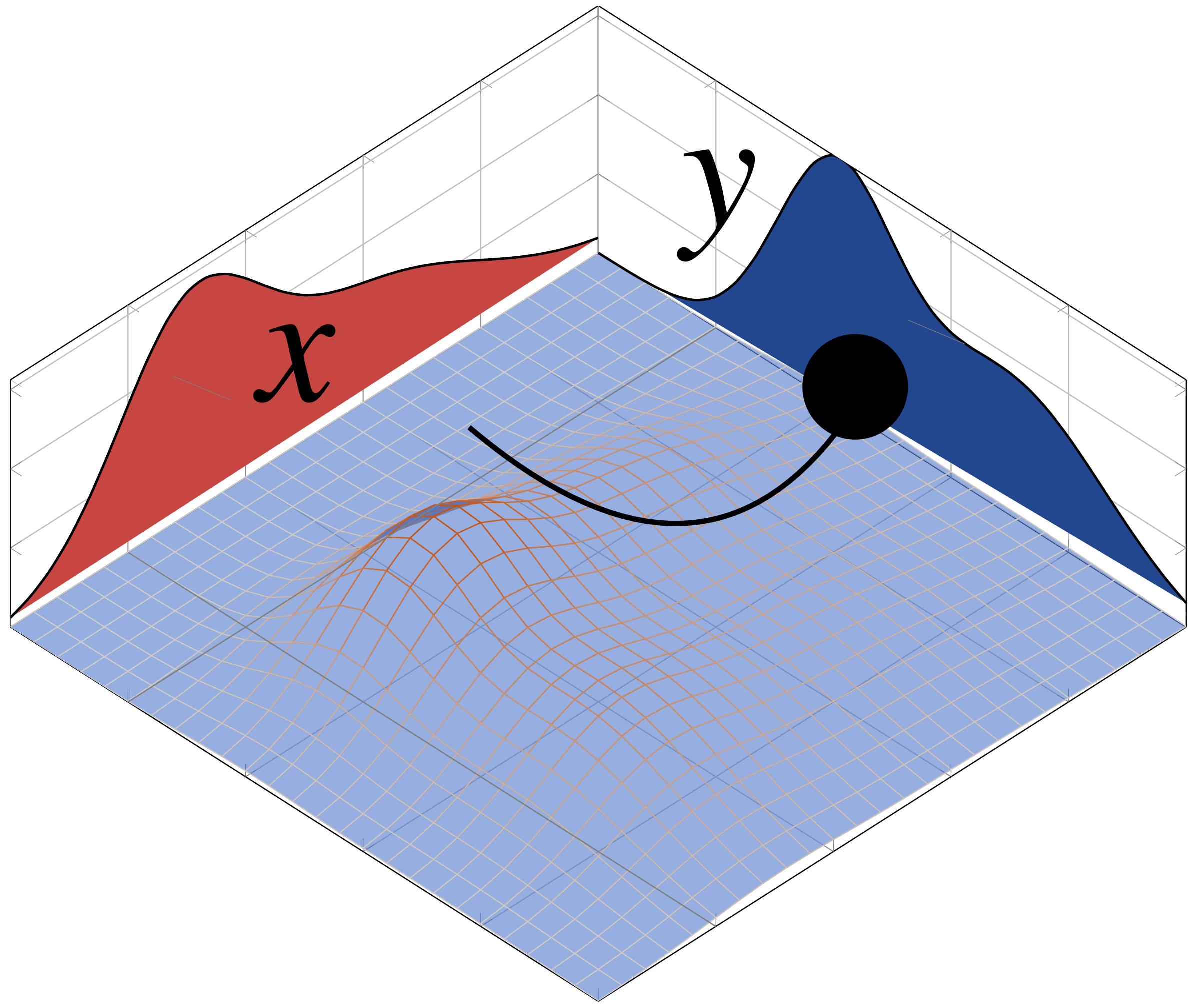
$$W_p^p(P, Q) := \inf \left\{ \int |x-y|^p \, d\Pi(x,y) \,\middle|\, \pi_\#^{(1)}\Pi = P,\ \pi_\#^{(2)}\Pi = Q \right\}$$

(**Dual Kantorovich problem**)

$$= \sup \left\{ \int \psi_1(x)\,\mathrm{d}P(x) + \int \psi_2(y)\,\mathrm{d}Q(y) \,\middle|\, \psi_1(x) + \psi_2(y) \leq |x-y|^p \right\}$$

2-Wasserstein space $(\mathrm{Prob}(\mathbb{R}^d), W_2)$ is a geodesic metric space.

Background: Wasserstein Geometry



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

$$W_p^p(P, Q) := \inf \left\{ \int |x - y|^p \, d\Pi(x, y) \,\middle|\, \pi_\#^{(1)}\Pi = P,\ \pi_\#^{(2)}\Pi = Q \right\}$$

(**Dual Kantorovich problem**)

$$= \sup \left\{ \int \psi_1(x)\, \mathrm{d}P(x) + \int \psi_2(y)\, \mathrm{d}Q(y) \,\middle|\, \psi_1(x) + \psi_2(y) \leq |x - y|^p \right\}$$

2-Wasserstein space $(\mathrm{Prob}(\mathbb{R}^d), W_2)$ is a geodesic metric space.

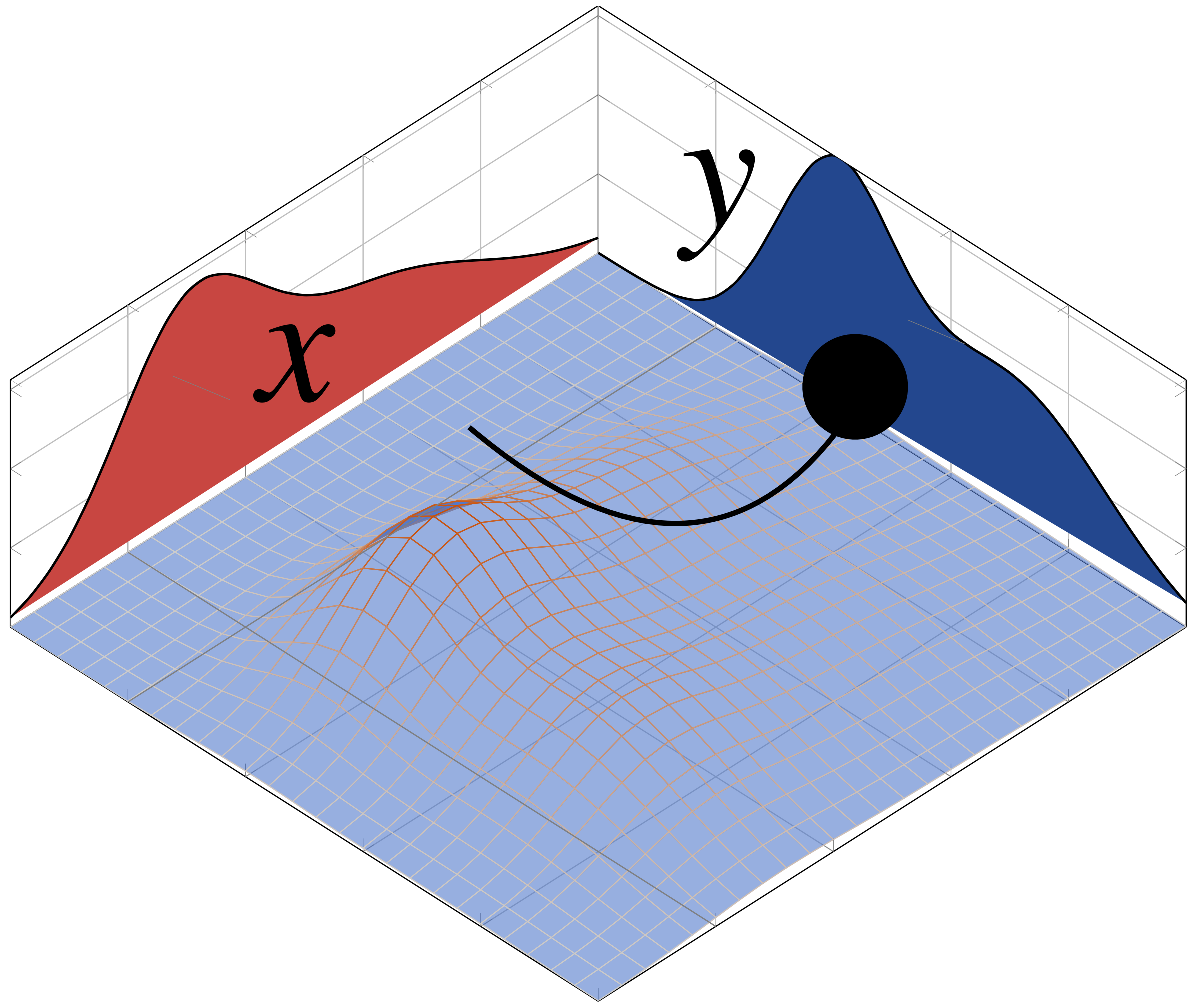
Dynamic formulation: *Benamou–Brenier*

$$W_2^2(P, Q) = \min \left\{ \int_0^1 \int |v_t|^2 \mathrm{d}\mu_t \mathrm{d}t \,\middle|\, \mu_0 = P, \mu_1 = Q, \frac{\mathrm{d}}{\mathrm{d}t}\mu_t + \mathrm{div}(v_t \mu_t) = 0 \right\}$$

Background: Wasserstein Geometry

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

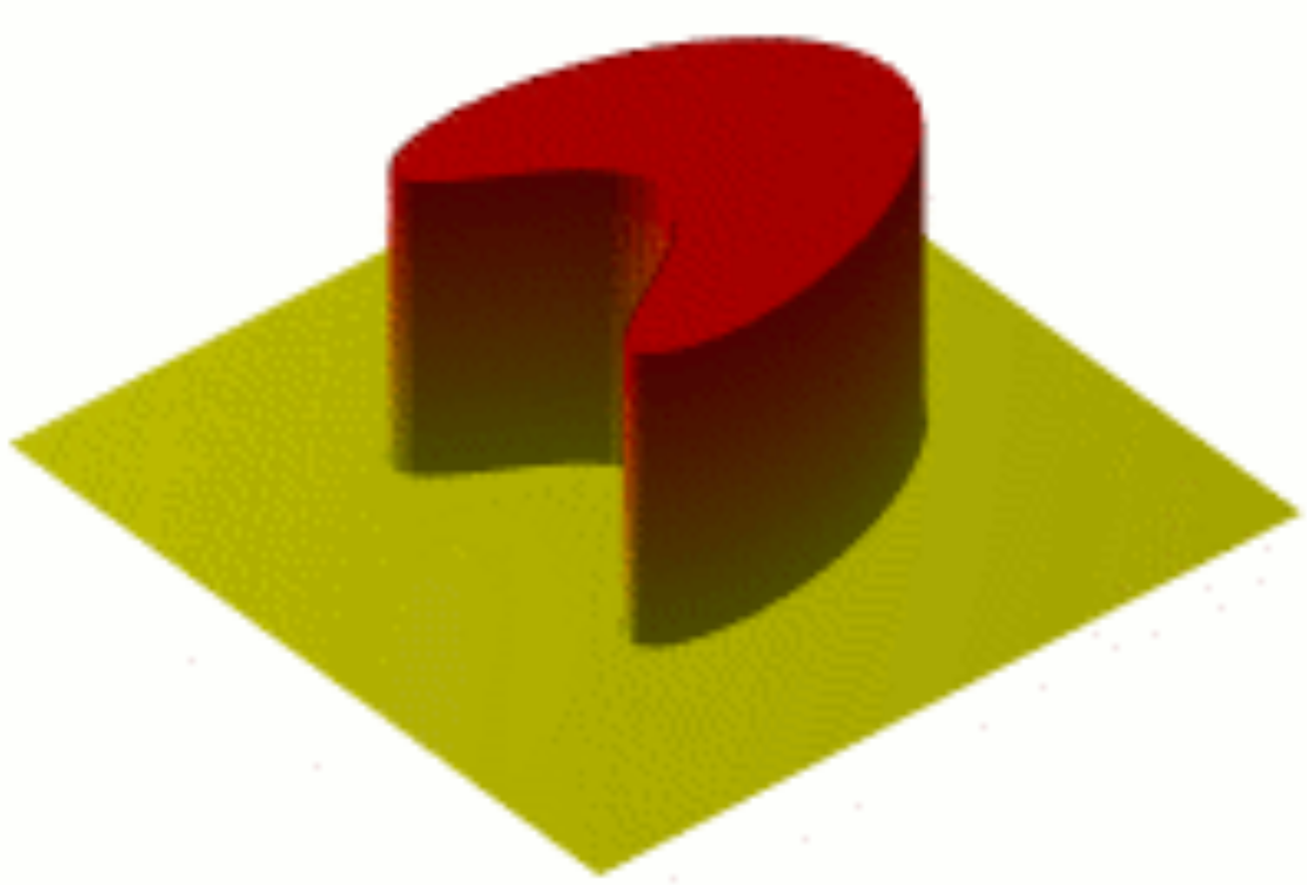
$$W_p^p(P, Q) := \inf \left\{ \int |x - y|^p \, d\Pi(x, y) \,\middle|\, \pi_\#^{(1)}\Pi = P,\ \pi_\#^{(2)}\Pi = Q \right\}$$



(**Dual Kantorovich problem**)

$$= \sup \left\{ \int \psi_1(x) \, \mathrm{d}P(x) + \int \psi_2(y) \, \mathrm{d}Q(y) \,\middle|\, \psi_1(x) + \psi_2(y) \leq |x - y|^p \right\}$$

2-Wasserstein space $(\mathrm{Prob}(\mathbb{R}^d), W_2)$ is a geodesic metric space.



Dynamic formulation: *Benamou–Brenier*

$$W_2^2(P, Q) = \min \left\{ \int_0^1 \int |v_t|^2 \mathrm{d}\mu_t \mathrm{d}t \,\middle|\, \mu_0 = P, \mu_1 = Q, \frac{\mathrm{d}}{\mathrm{d}t}\mu_t + \mathrm{div}(v_t \mu_t) = 0 \right\}$$

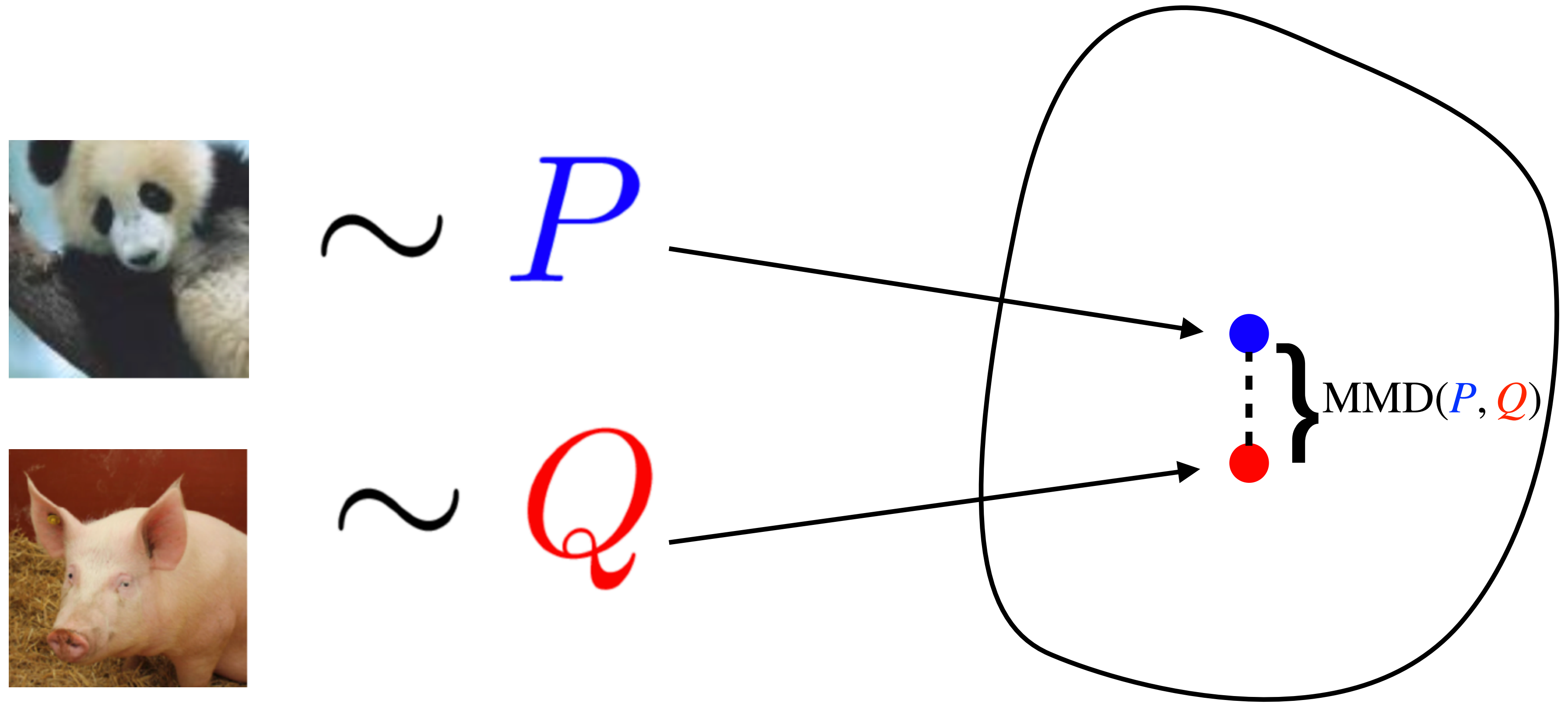
Background: “Kernel Geometry”

Background: “Kernel Geometry”

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.



Background: "Kernel Geometry"

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

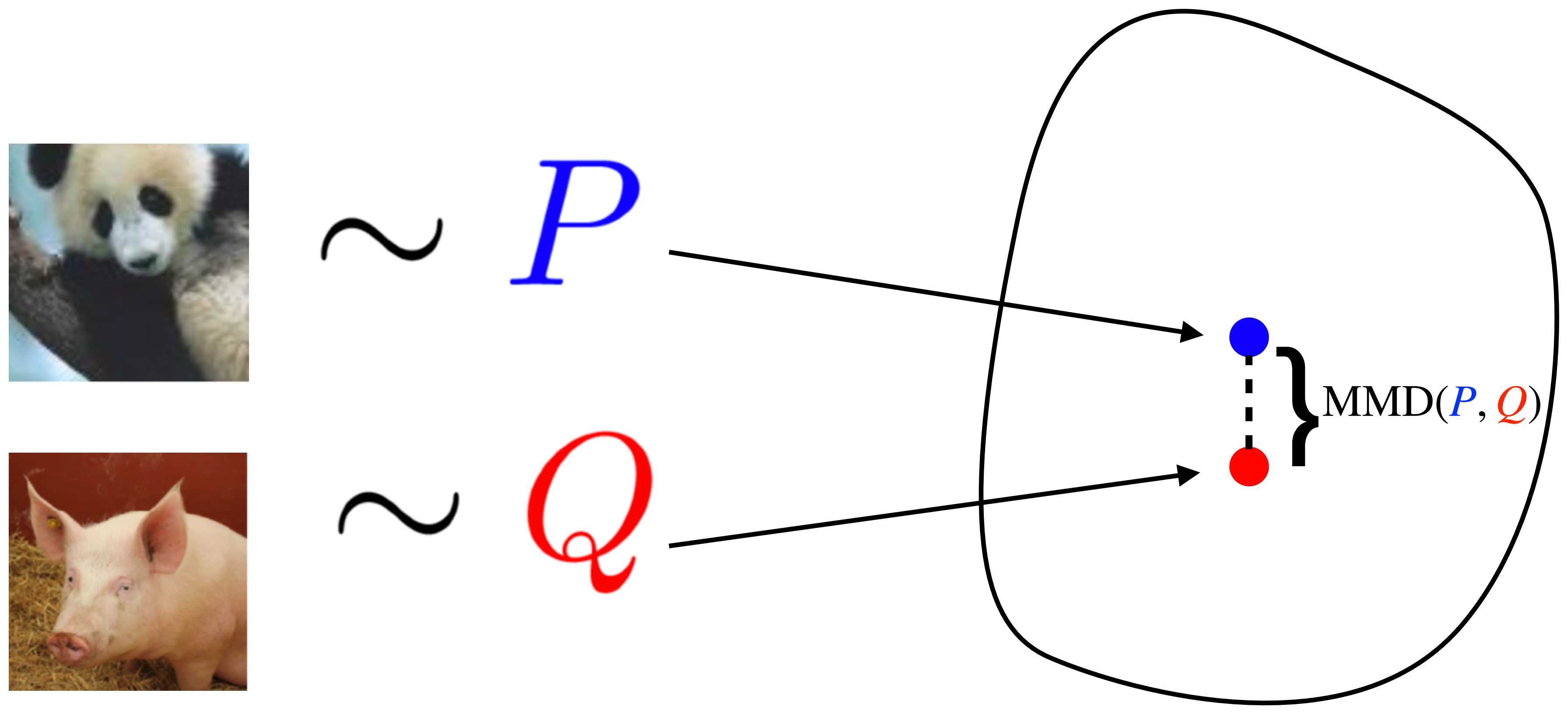
$$\mathrm{MMD}(P, Q) := \left\| \int k(x, \cdot\,) dP - \int k(x, \cdot\,) dQ \right\|_{\mathcal{H}}.$$

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

Dual formulation as an integral probability metric.

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

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



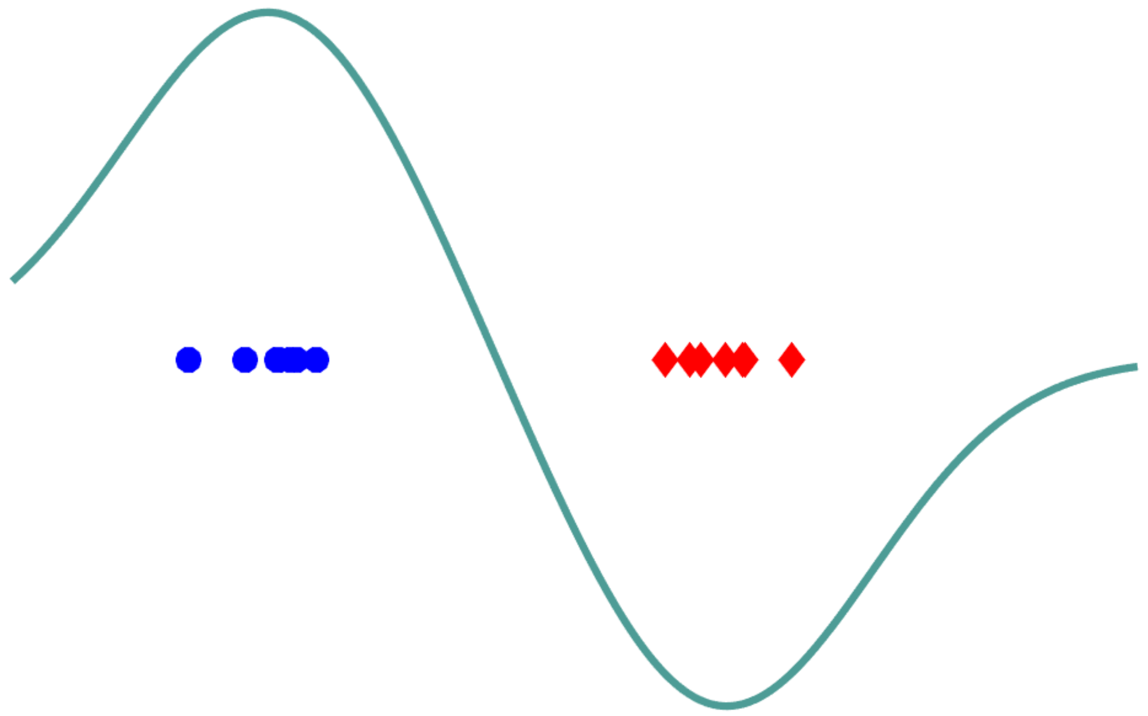


Figure credit: W. Jitkrittum, J. Zhu

Background: “Kernel Geometry”

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

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

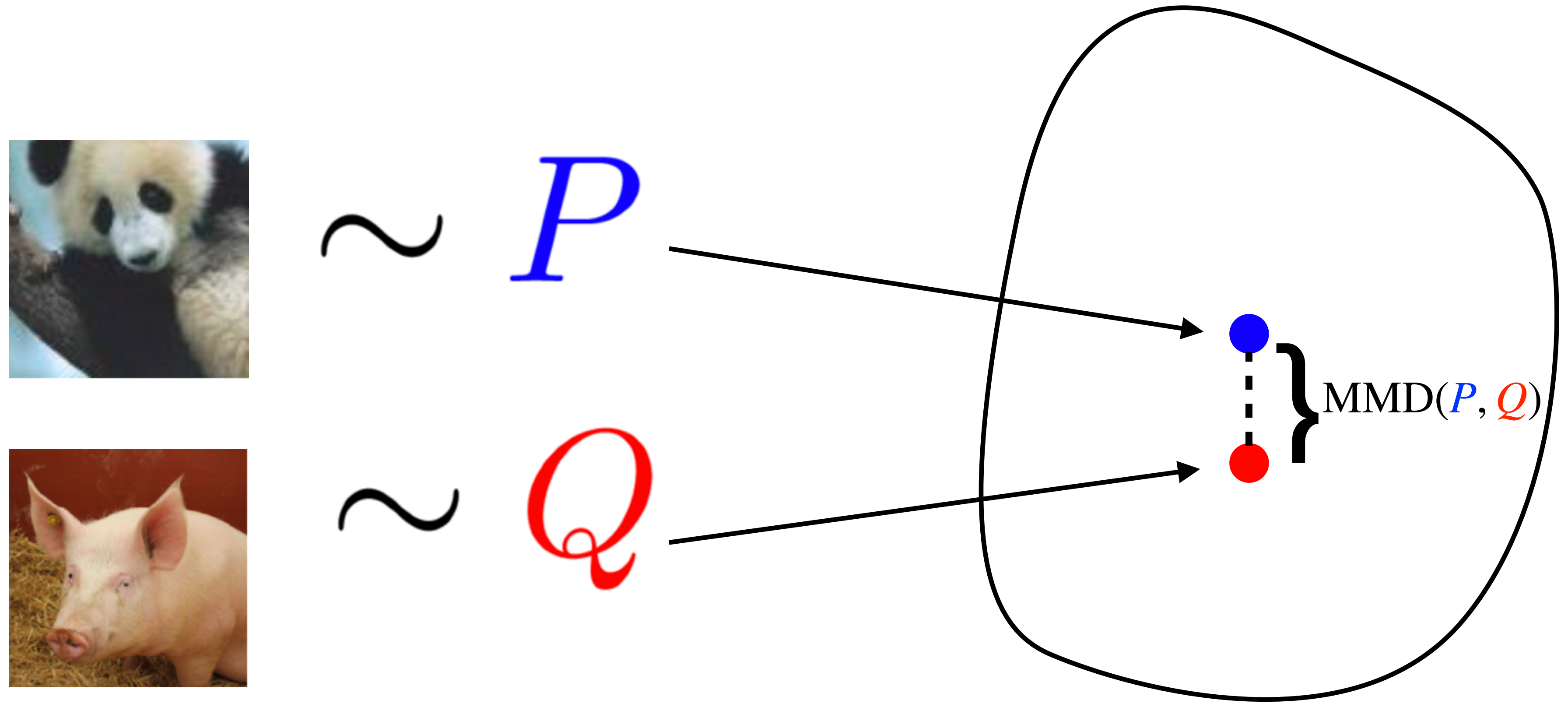
$(\mathrm{Prob}(\mathbb{R}^d), \mathrm{MMD})$ is a (simple) metric space.

Dual formulation as an integral probability metric.

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

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

Example. Approx. nonlinear functions



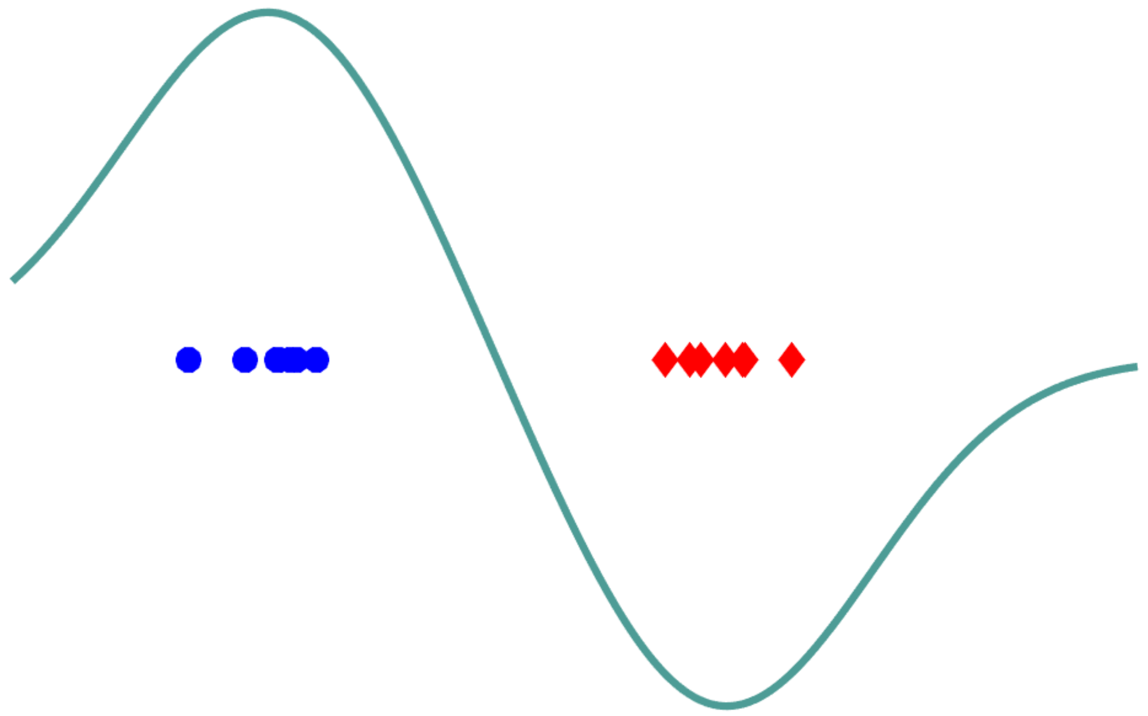


Figure credit: W. Jitkrittum, J. Zhu

Background: "Kernel Geometry"

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.

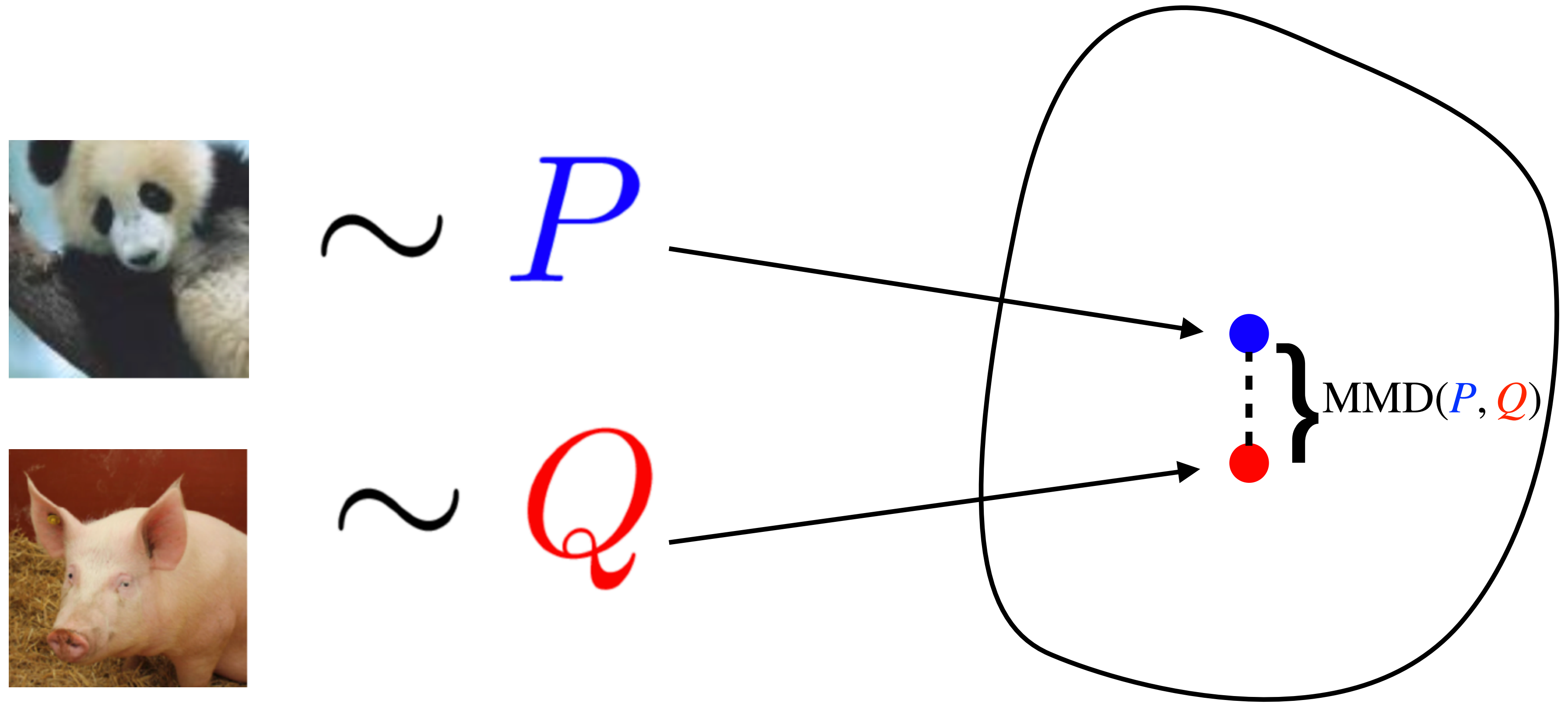
Dual formulation as an integral probability metric.

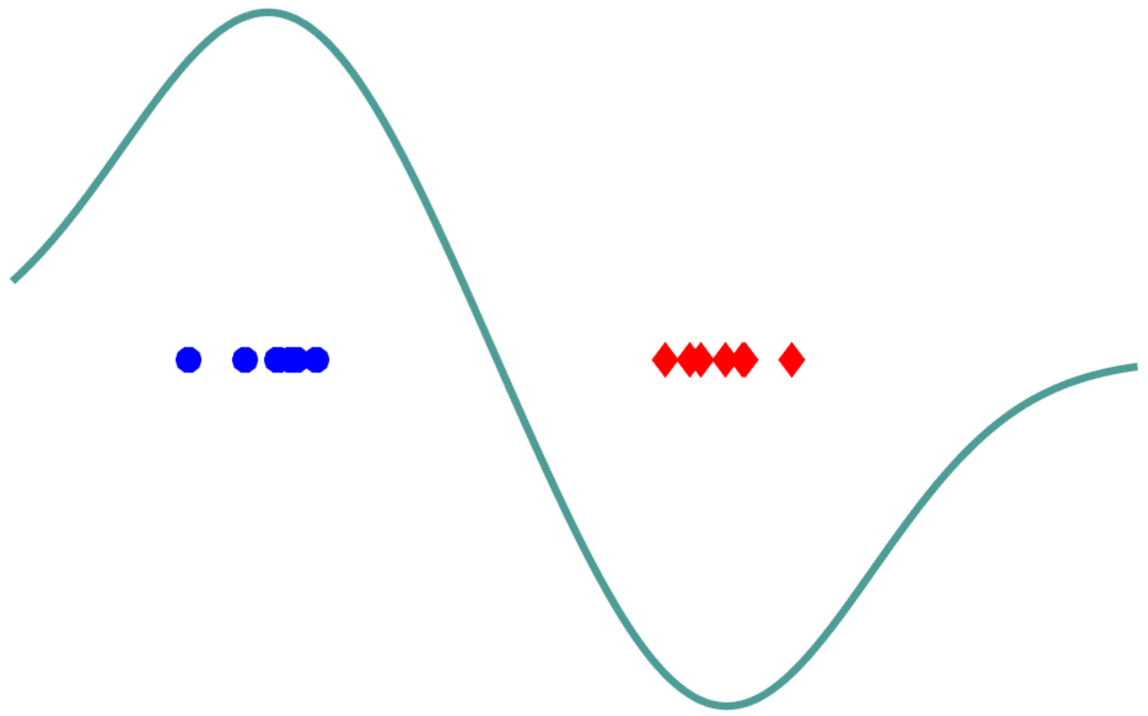
$$\mathrm{MMD}(P, Q) = \sup_{\|f\|_{\mathscr{H}} \le 1} \int f \, d(P - Q)$$

$\mathscr{H}$ 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 $\mathscr{H}$.

Example. Approx. nonlinear functions

$$\min_{f \in \mathscr{H}} \frac{1}{N} \sum_{i=1}^{N} \|f(x_i) - y_i\|^2 + \lambda \|f\|_{\mathscr{H}}^2$$





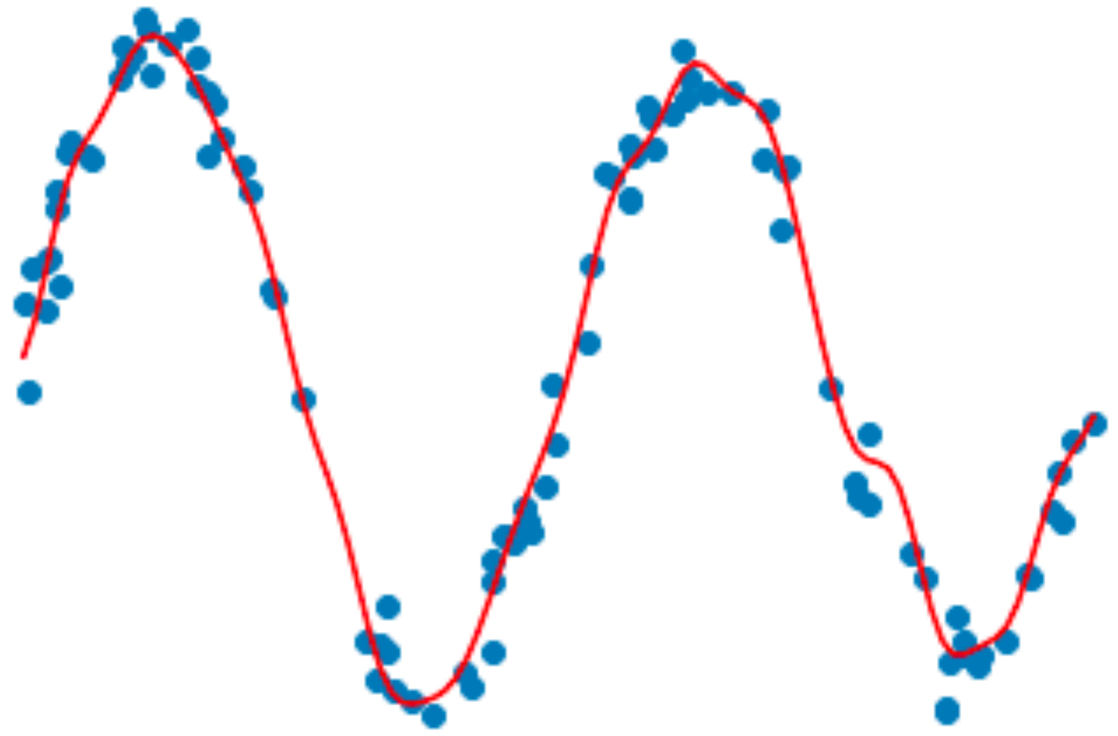


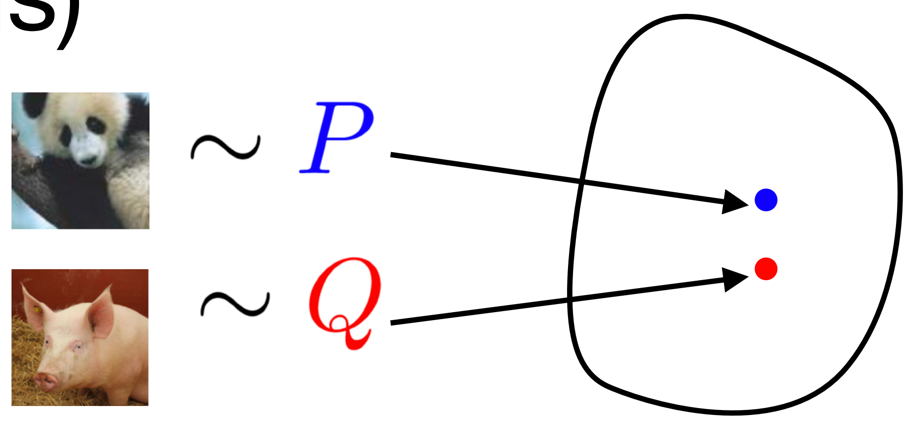
Figure credit: W. Jitkrittum, J. Zhu

Previous work: Kernel DRO

Previous work: Kernel DRO

Primal DRO (not solvable as it is)

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



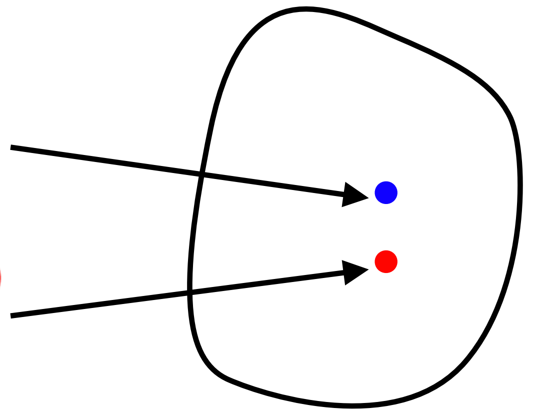
Previous work: Kernel DRO

Primal DRO (not solvable as it is)

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

 $\sim P$

 $\sim Q$



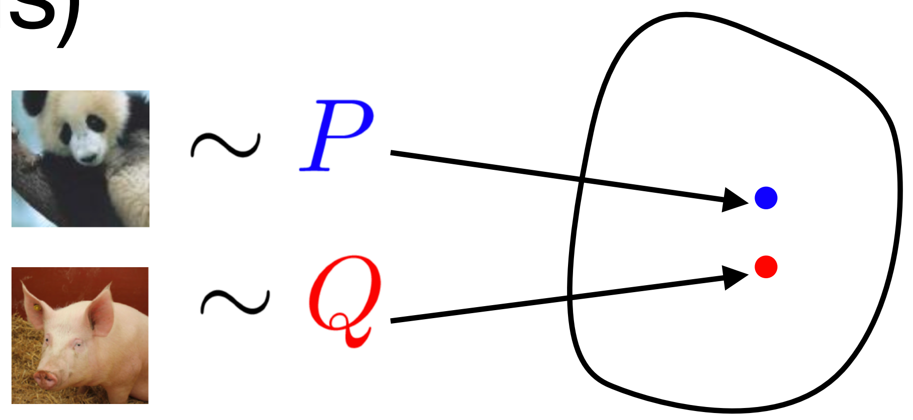
Kernel DRO Theorem (simplified). [Z. et al. 2021]
DRO problem is equivalent to the dual kernel machine learning problem, i.e., (DRO)=(K).

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

Previous work: Kernel DRO

Primal DRO (not solvable as it is)

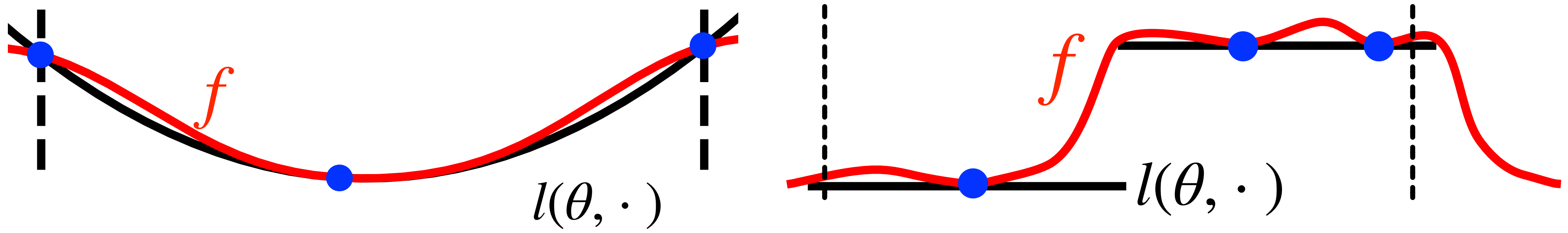
(DRO) $$\min_{\theta} \sup_{\mathrm{MMD}(Q,\hat{P})\leq\epsilon} \mathbb{E}_Q l(\theta, \xi)$$



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

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

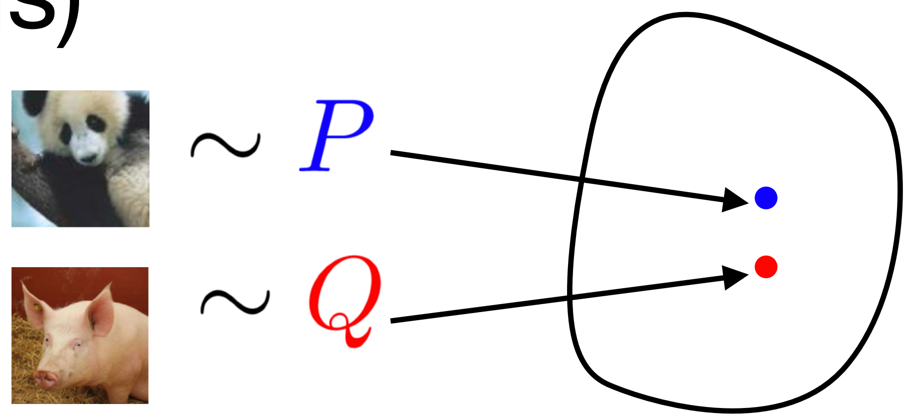
Geometric intuition: **dual kernel function f** as robust surrogate losses (flatten the curve)



Previous work: Kernel DRO

Primal DRO (not solvable as it is)

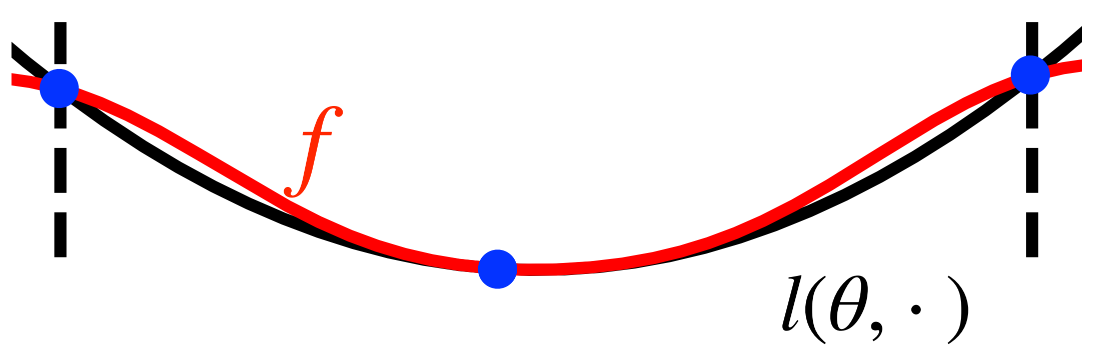
$$\text{(DRO)} \quad \min_{\theta} \sup_{\mathrm{MMD}(Q,\hat{P})\le\epsilon} \mathbb{E}_Q l(\theta,\xi)$$

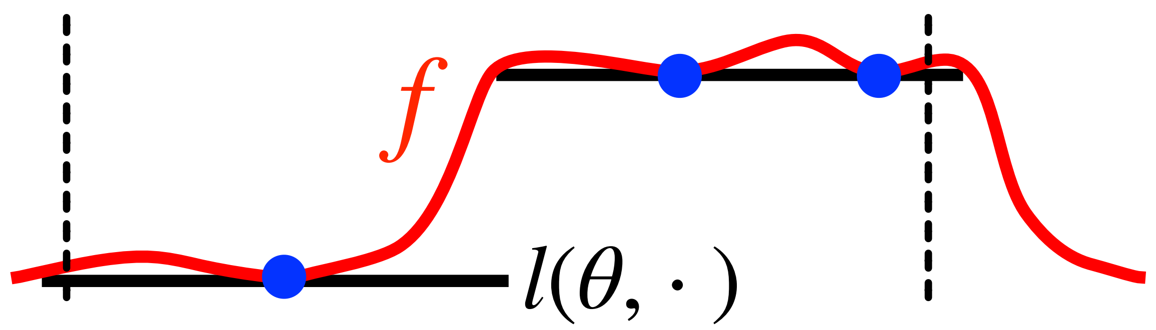


Kernel DRO Theorem (simplified). [Z. et al. 2021]
DRO problem is equivalent to the dual kernel machine learning problem, i.e., (DRO)=(K).

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

Geometric intuition: **dual kernel function f** as robust surrogate losses (flatten the curve)

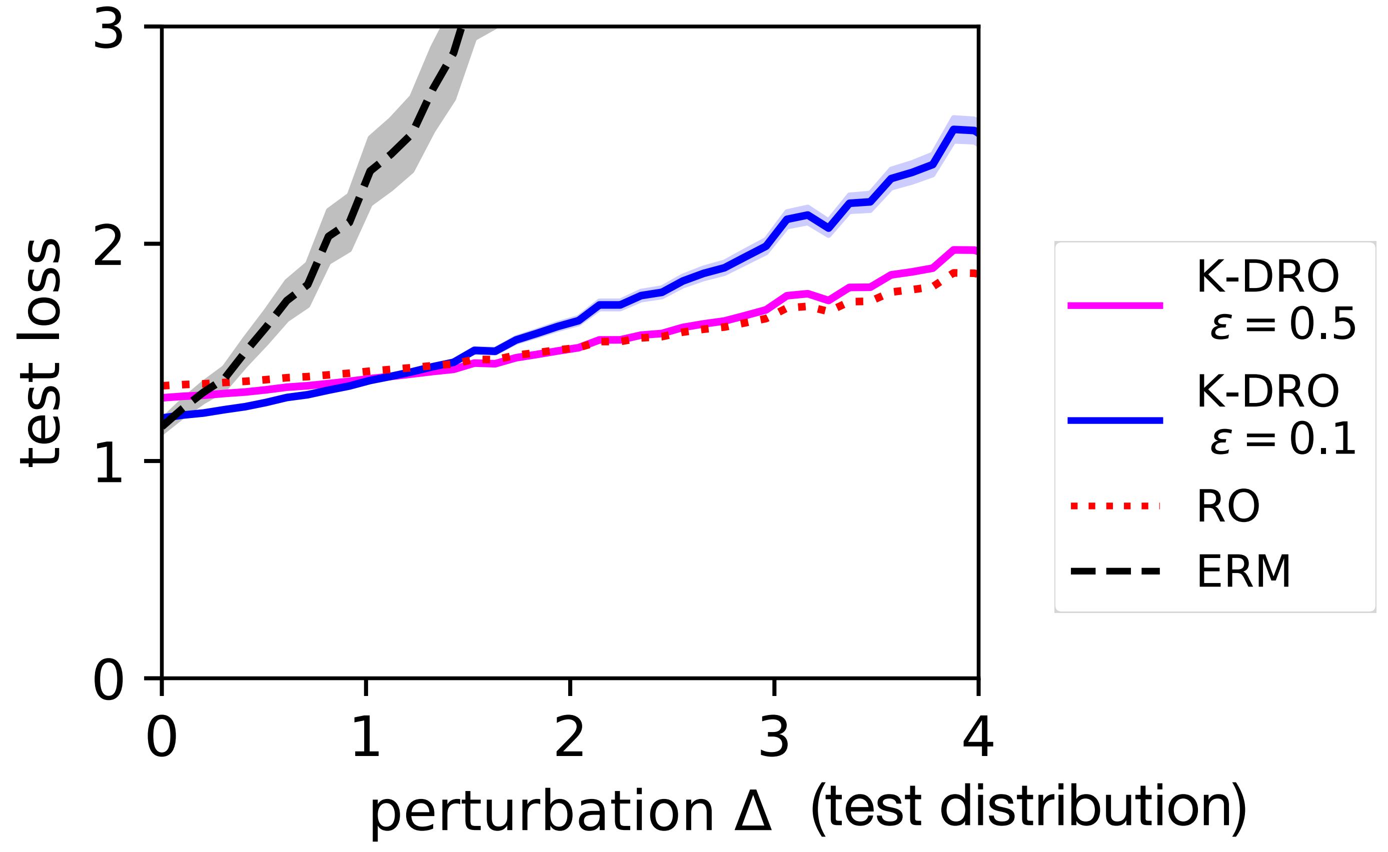




Example. Robust least squares
[El Ghaoui Lebret '97]

$$\text{minimize } l(\theta,\xi) := \|A(\xi)\cdot\theta - b\|_2^2$$

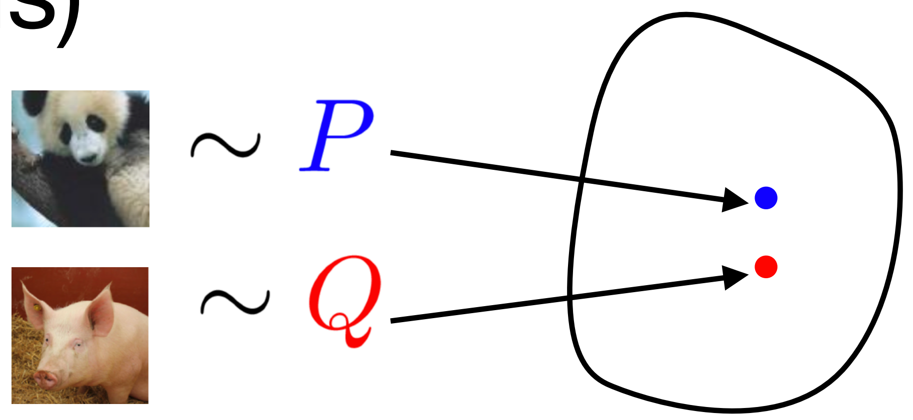
Given historical samples $\xi_1, \xi_2, \ldots, \xi_N$



Previous work: Kernel DRO

Primal DRO (not solvable as it is)

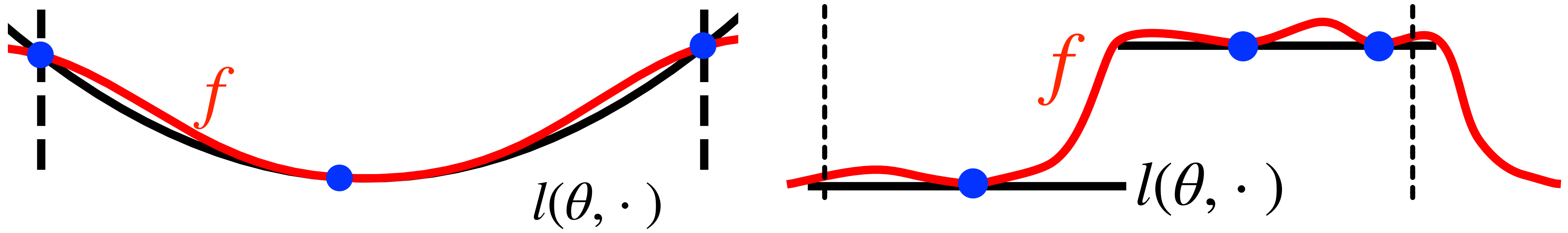
$$\text{(DRO)}\quad \min_{\theta} \sup_{\mathrm{MMD}(Q,\hat{P})\le\epsilon} \mathbb{E}_Q l(\theta,\xi)$$



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

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

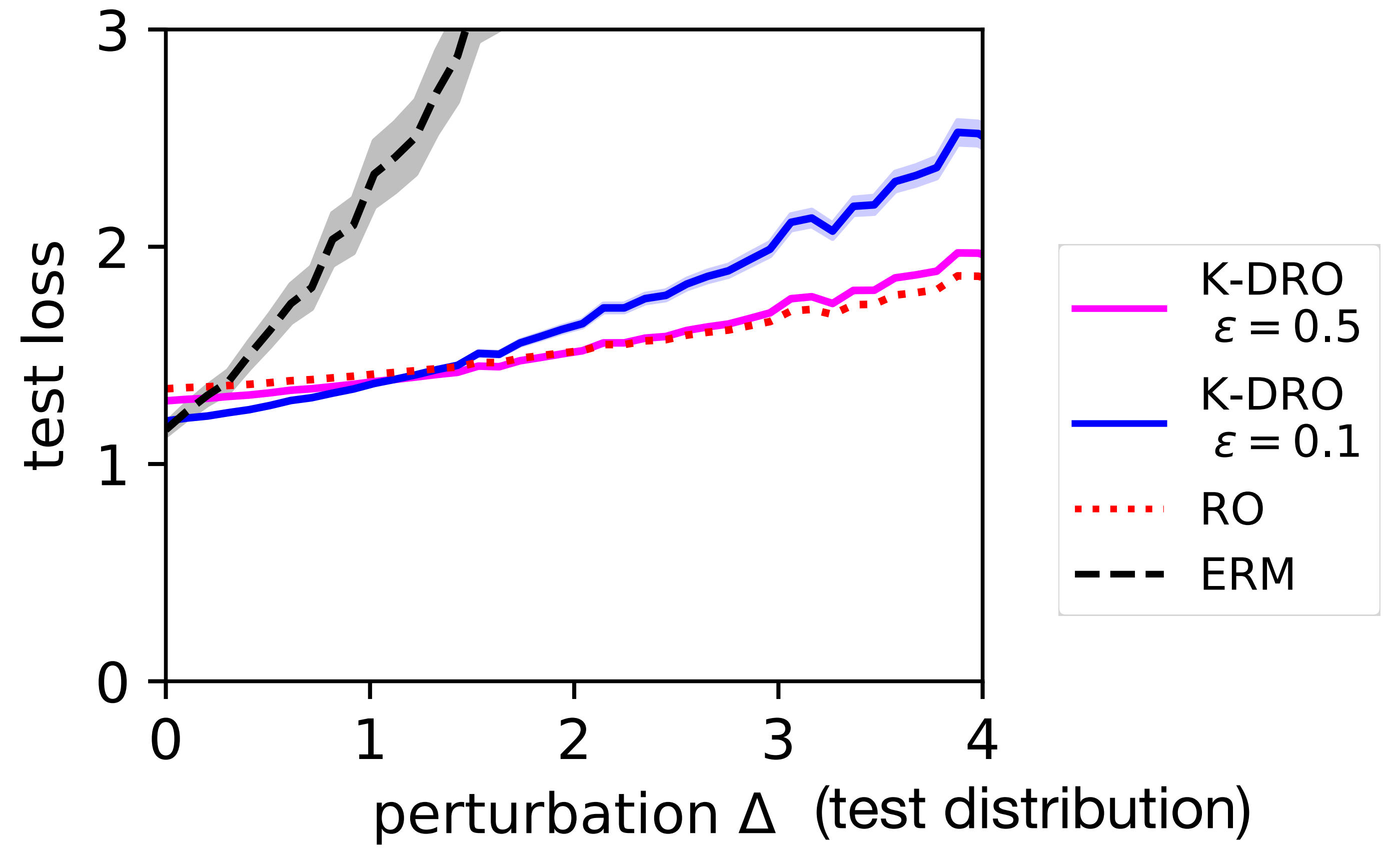
Geometric intuition: **dual kernel function f** as robust surrogate losses (<u>flatten the curve</u>)



Example. Robust least squares
[El Ghaoui Lebret '97]

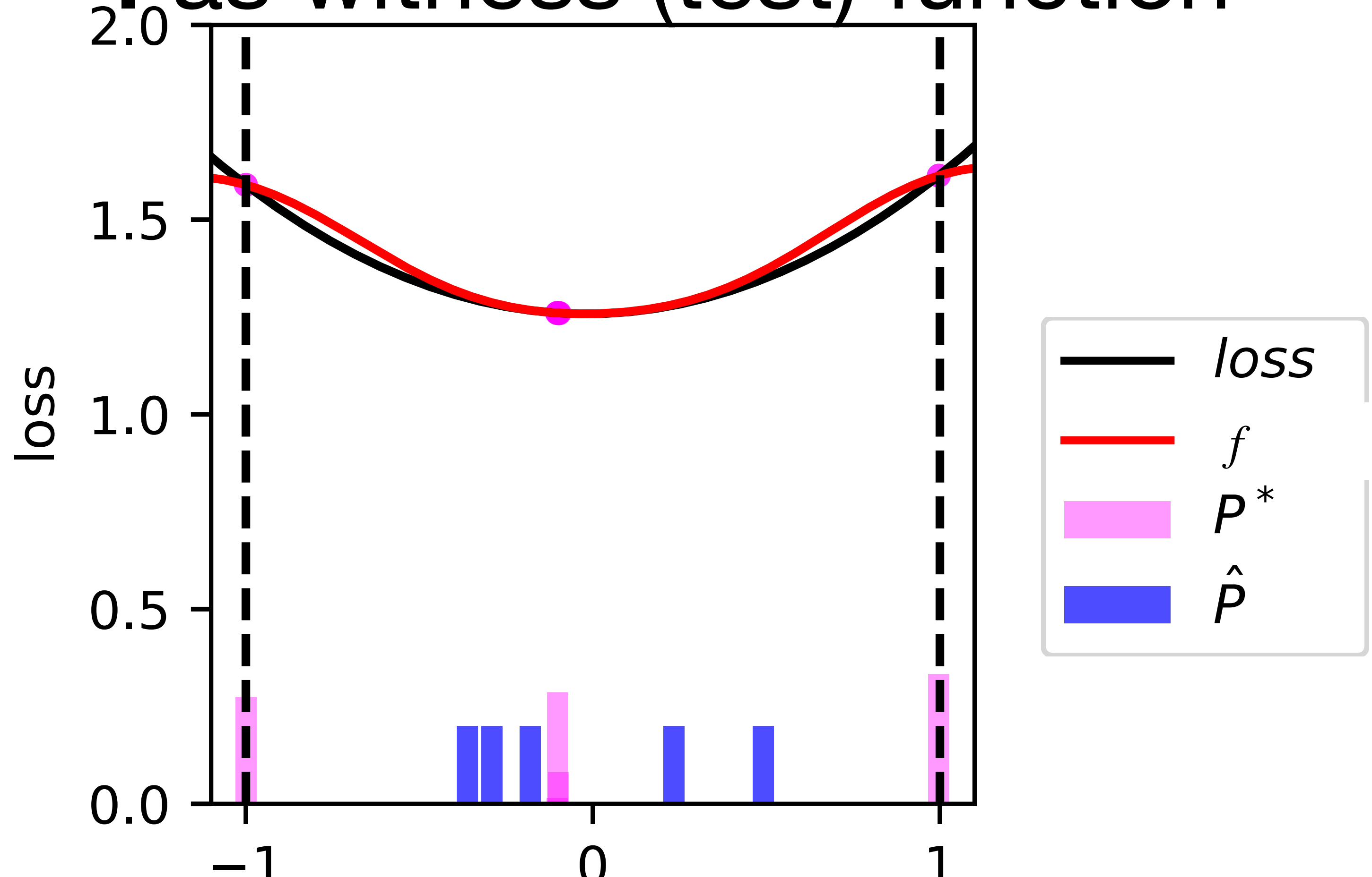
$$\text{minimize } l(\theta,\xi) := \|A(\xi)\cdot\theta - b\|_2^2$$

Given historical samples $\xi_1, \xi_2, \ldots, \xi_N$



Robustifying with DRO

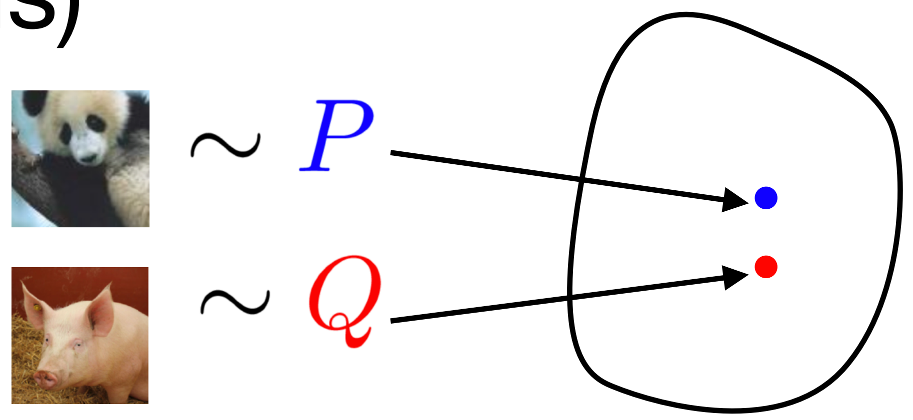
f as witness (test) function



Previous work: Kernel DRO

Primal DRO (not solvable as it is)

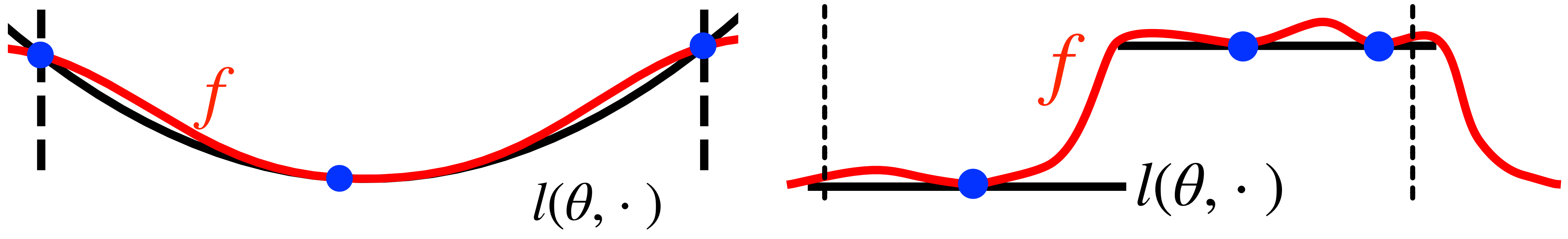
$$\text{(DRO)} \quad \min_{\theta} \sup_{\mathrm{MMD}(Q,\hat{P})\le\epsilon} \mathbb{E}_Q l(\theta,\xi)$$



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

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

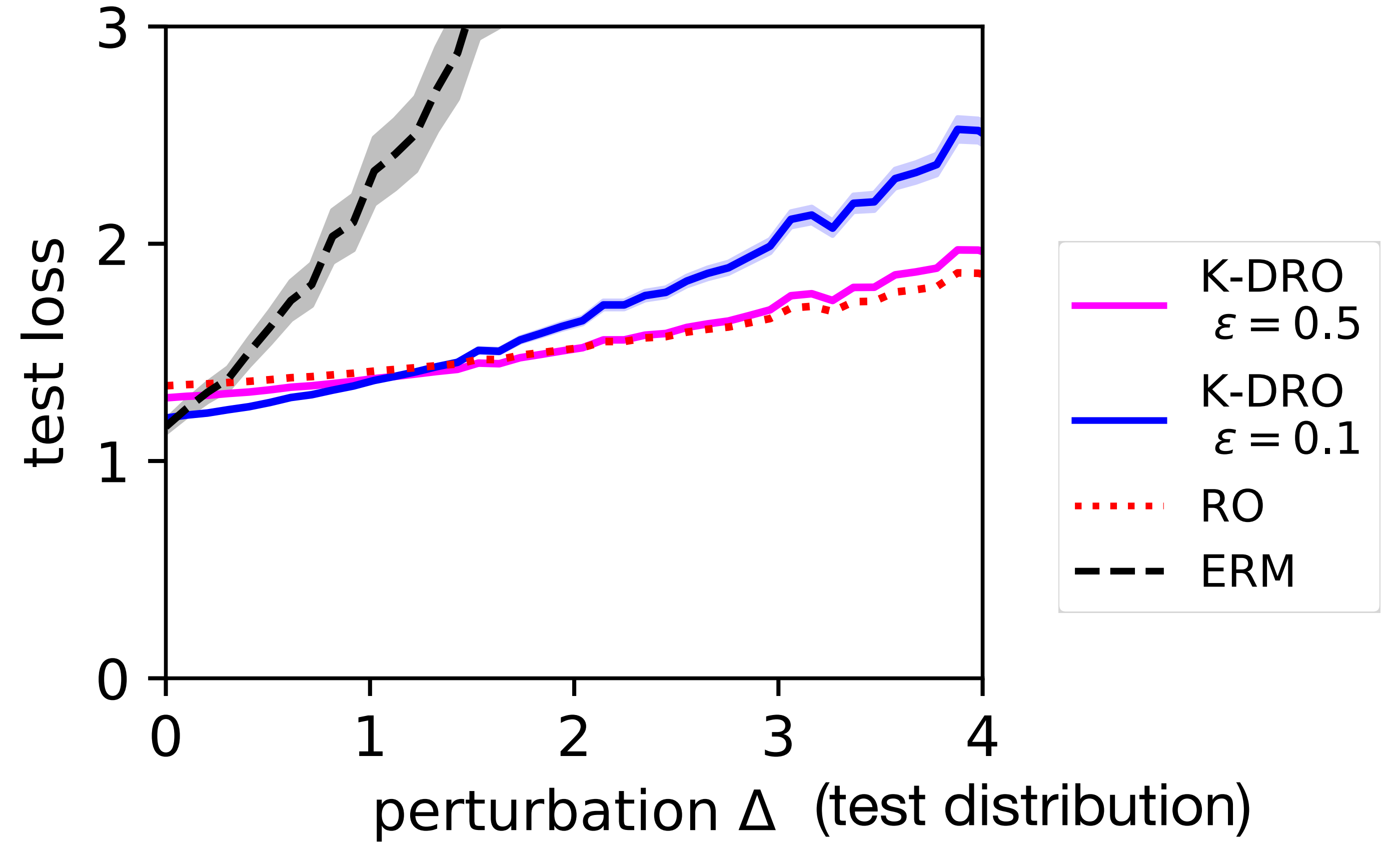
Geometric intuition: **dual kernel function f** as robust surrogate losses (flatten the curve)



Example. Robust least squares
[El Ghaoui Lebret '97]

$$\text{minimize } l(\theta,\xi) := \|A(\xi)\cdot\theta - b\|_2^2$$

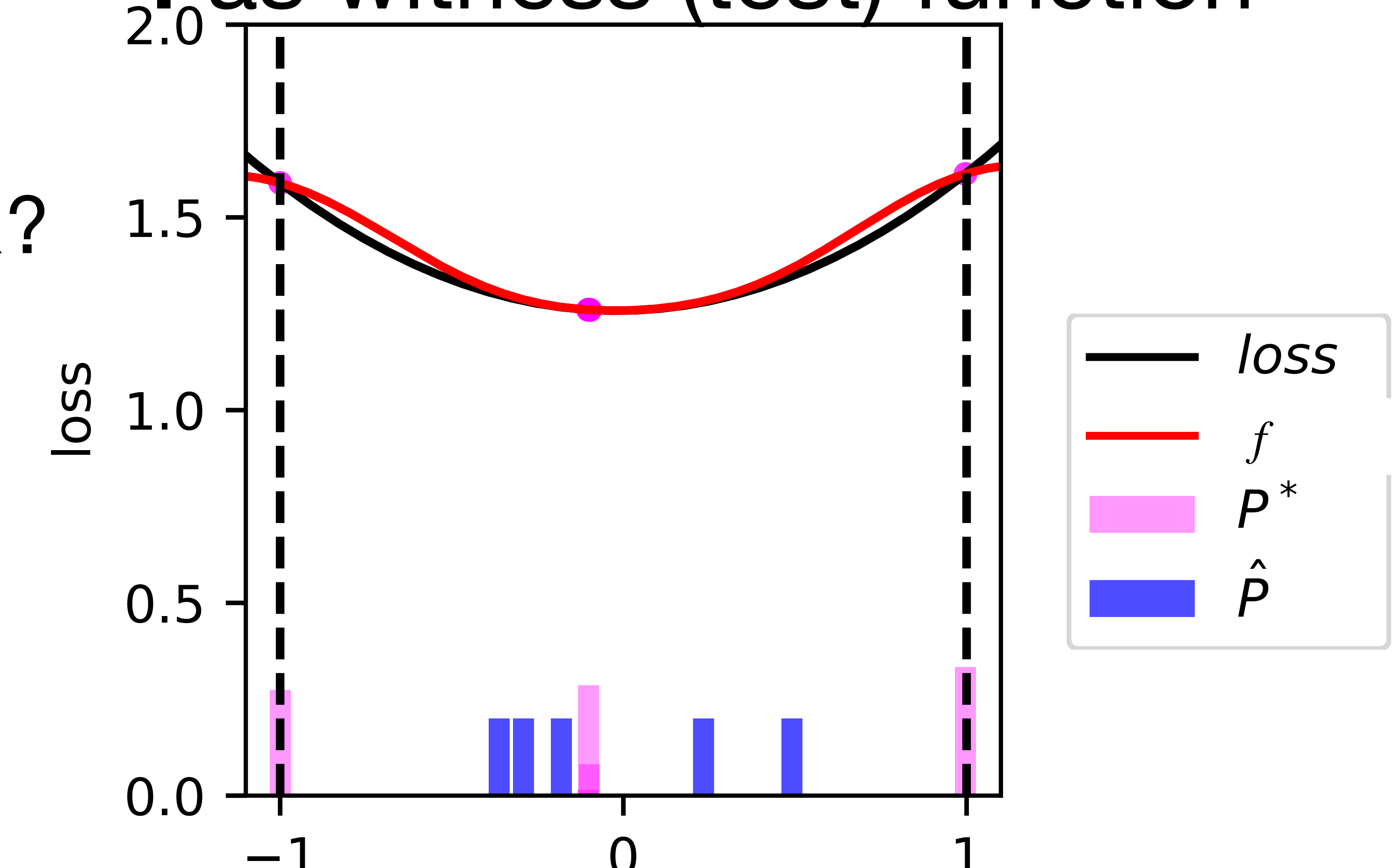
Given historical samples $\xi_1, \xi_2, \ldots, \xi_N$



Robustifying with DRO

f as witness (test) function

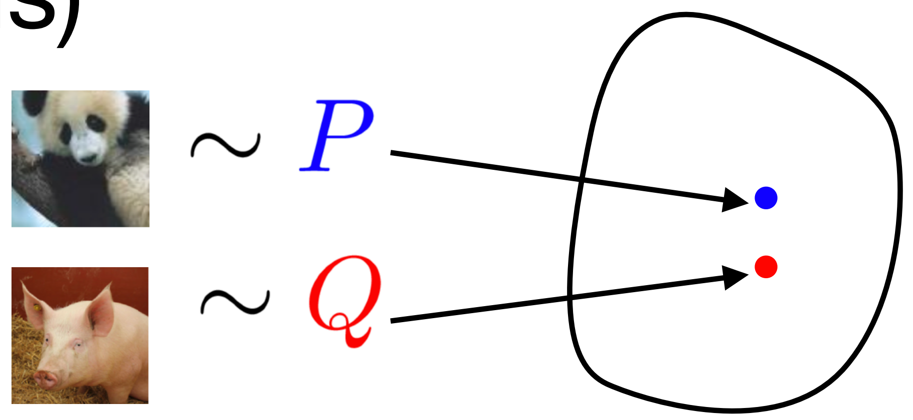
What if $f \equiv c \in \mathbb{R}$?



Previous work: Kernel DRO

Primal DRO (not solvable as it is)

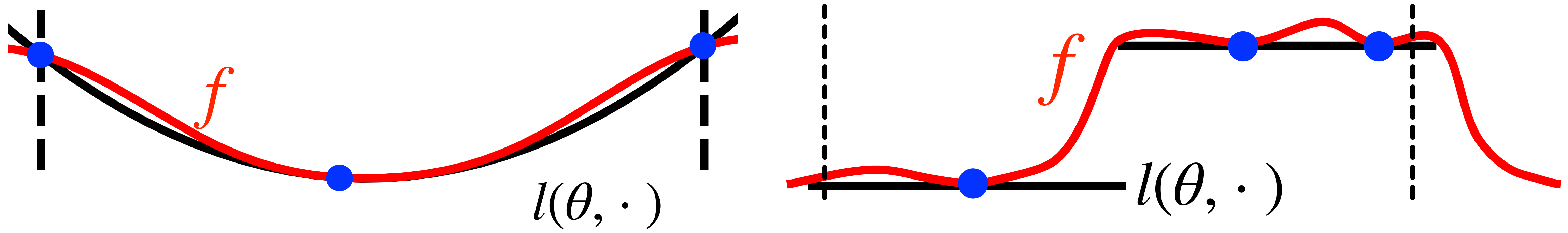
$$\text{(DRO)} \quad \min_{\theta} \sup_{\mathrm{MMD}(Q,\hat{P})\le\epsilon} \mathbb{E}_Q l(\theta,\xi)$$



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

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

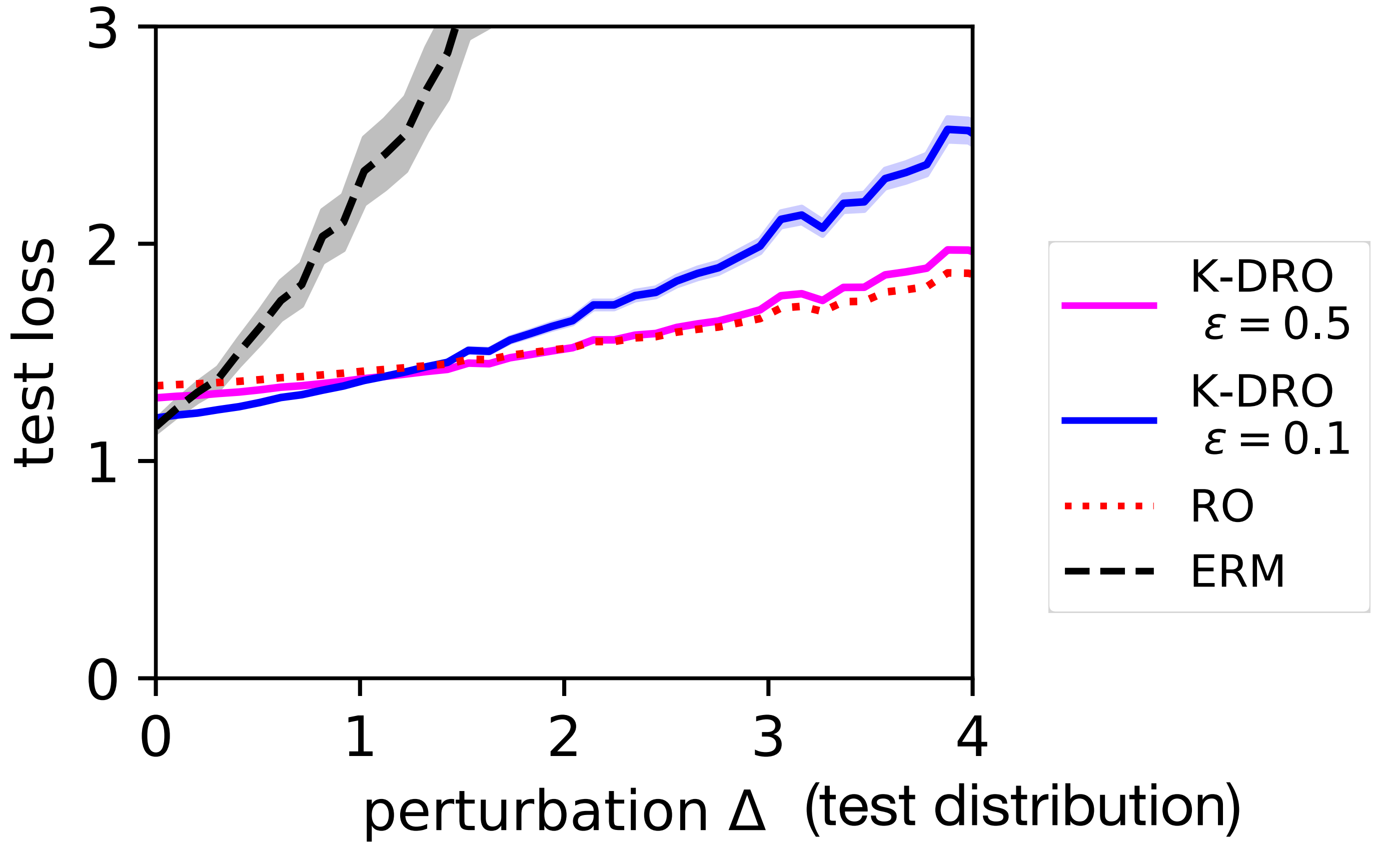
Geometric intuition: **dual kernel function f** as robust surrogate losses (flatten the curve)



Example. Robust least squares
[El Ghaoui Lebret '97]

$$\text{minimize } l(\theta,\xi) := \|A(\xi)\cdot\theta - b\|_2^2$$

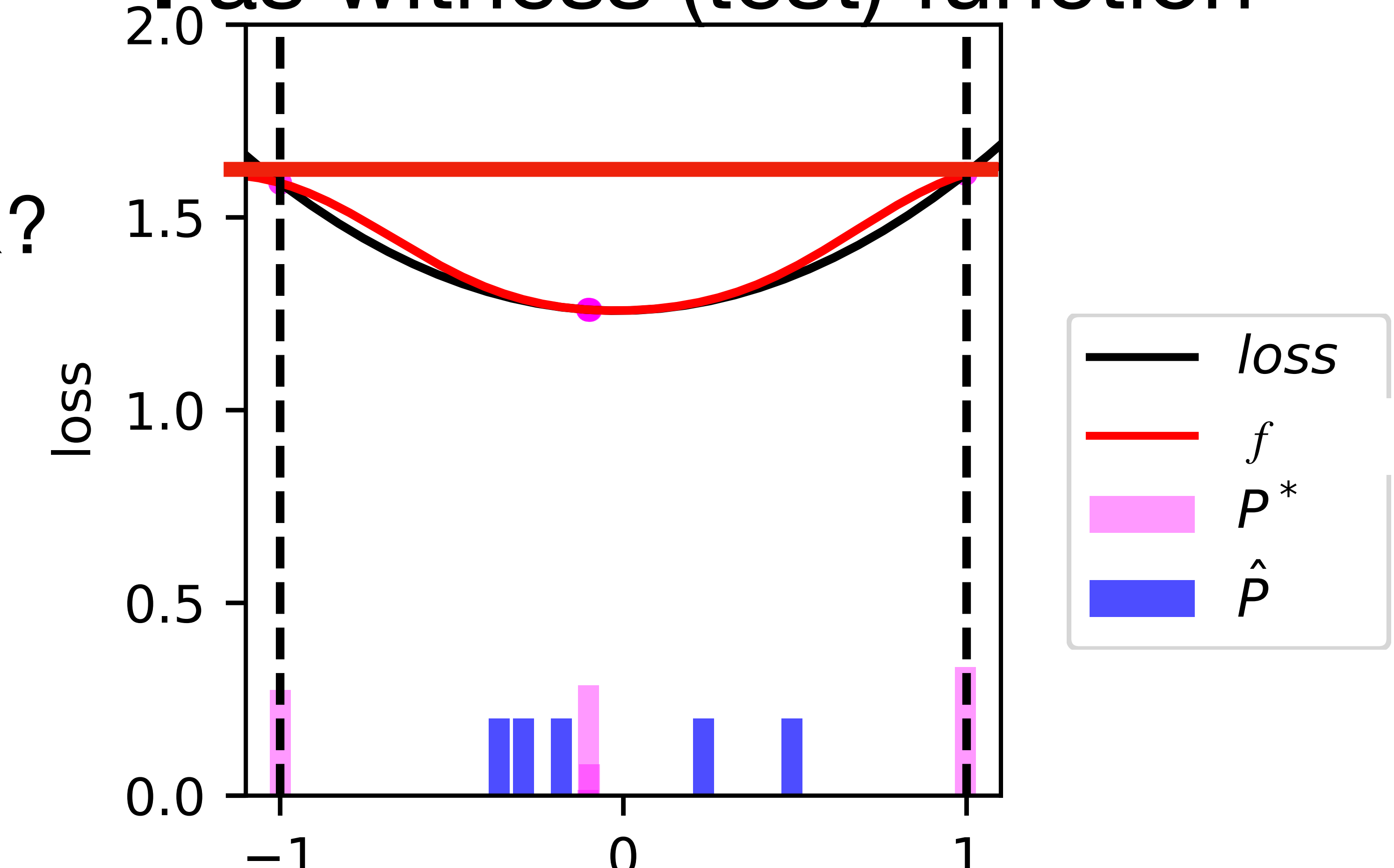
Given historical samples $\xi_1, \xi_2, \ldots, \xi_N$



Robustifying with DRO

f as witness (test) function

What if $f \equiv c \in \mathbb{R}$?



Duality perspective

Duality perspective

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]

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

Duality perspective

2-Wasserstein

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

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

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

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

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

Duality perspective

2-Wasserstein

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

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

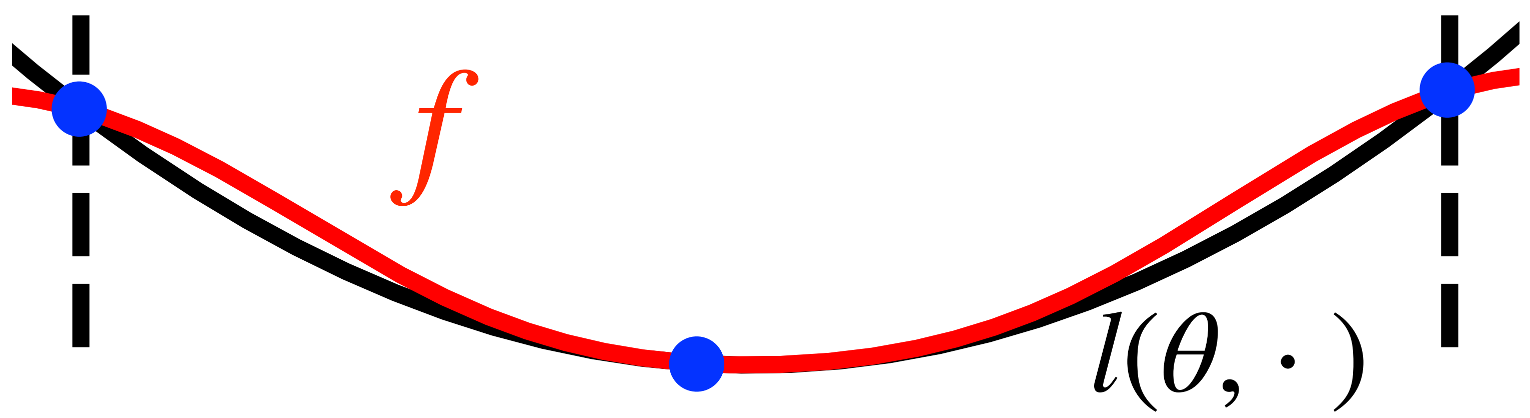
where Moreau envelope
$$l_\theta^{\lambda\|\cdot\|^2}(x) := \sup_u l(\theta,u) - \lambda\|u-x\|^2$$

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

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

Dual: $$\min_{\theta,f\in\mathcal{H}} \frac{1}{N}\sum_{i=1}^{N} f(\xi_i) + \epsilon\|f\|_{\mathcal{H}}$$

$$\text{s.t. } l(\theta,\xi) \le f(\xi), \forall\xi \text{ a.e.}$$



Duality perspective

2-Wasserstein

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

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

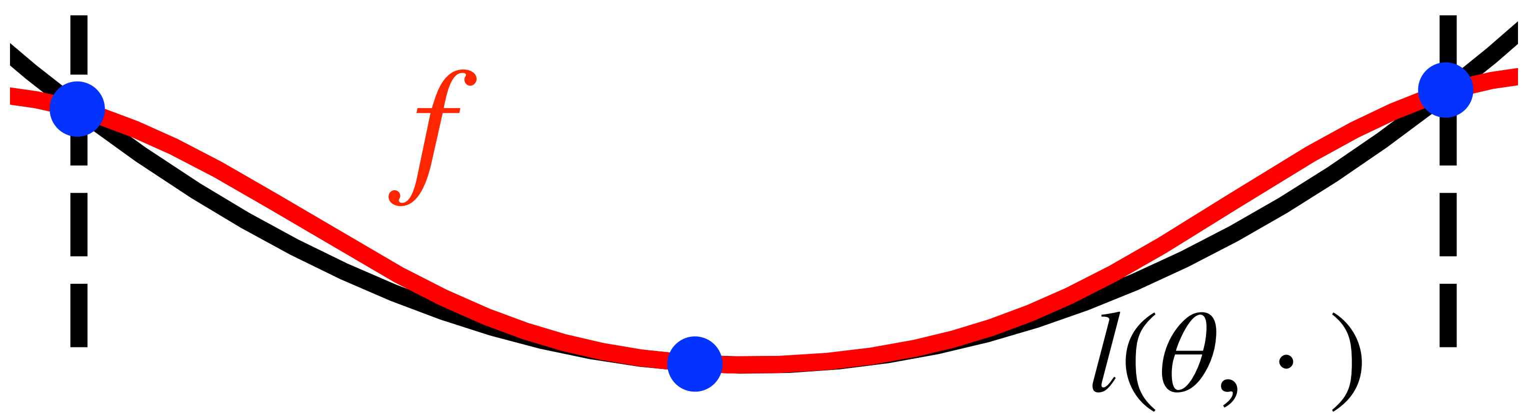
- l is **nonconvex** (e.g., DNN, g-non-cvx)
- **Nonlinear (in measure)** energies

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

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

Dual: $$\min_{\theta, f\in\mathscr{H}} \frac{1}{N}\sum_{i=1}^{N} f(\xi_i) + \epsilon\|f\|_{\mathscr{H}}$$

$$\text{s.t. } l(\theta,\xi) \le f(\xi), \forall \xi \text{ a.e.}$$



Duality perspective

2-Wasserstein

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

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

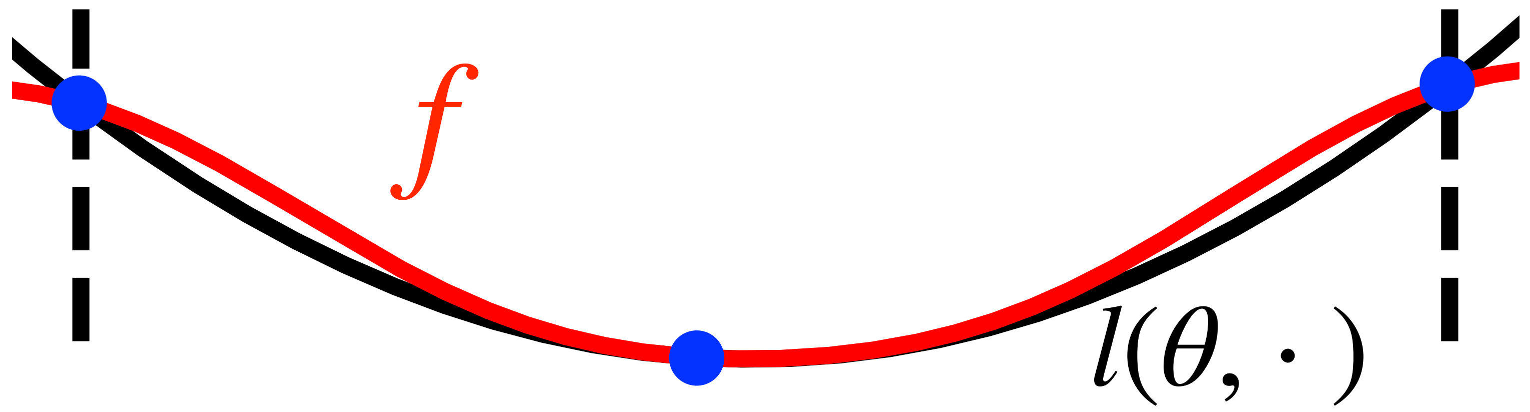
- l is **nonconvex** (e.g., DNN, g-non-cvx)
- **Nonlinear (in measure)** energies

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

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

Dual: $$\min_{\theta,f\in\mathscr{H}} \frac{1}{N}\sum_{i=1}^{N} f(\xi_i) + \epsilon\|f\|_{\mathscr{H}}$$

$$\text{s.t.}\ \ l(\theta,\xi) \le f(\xi), \forall\xi \text{ a.e.}$$



Nonlinear kernel approx. as robust surrogate losses (<u>flatten the curve</u>)

Duality of
Gradient Flow Force-Balance

From static DRO to JKO scheme for gradient flows

DRO's Wasserstein measure optimization is not new.

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

$$\min_{\theta} \sup_{P} \mathbb{E}_P\, l(\theta, \xi) - \gamma \cdot W_2^2(P, \hat{P})$$

From static DRO to JKO scheme for gradient flows

DRO's Wasserstein measure optimization is not new.

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

$$\min_{\theta} \sup_{P} \mathbb{E}_P\, l(\theta,\xi) - \gamma \cdot W_2^2(P,\hat{P})$$

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

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

is the gradient-flow equation of energy F in $(\mathrm{Prob}(\bar{X}), W_2)$.

From static DRO to JKO scheme for gradient flows

DRO's Wasserstein measure optimization is not new.

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

$$\min_{\theta} \sup_{P} \mathbb{E}_P\, l(\theta,\xi) - \gamma \cdot W_2^2(P,\hat{P})$$

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

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

is the gradient-flow equation of energy F in $(\mathrm{Prob}(\bar{X}), W_2)$.

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.

Duality in gradient flow dynamics: ODE

$$\dot{x}(t) = -\nabla f(x(t))$$

Duality in gradient flow dynamics: ODE

$$\dot{x}(t) = -\nabla f(x(t))$$

$\dot{x}(t) \in X$ provides the **rate (or velocity)** (we can see)

Duality in gradient flow dynamics: ODE

$$\dot{x}(t) = -\nabla f(x(t))$$

$\dot{x}(t) \in X$ provides the **rate (or velocity)** (we can see)

$-\nabla f(x(t)) \in X^*$ provides the **(thermodynamic) force** (can't see; shadow price)

Duality in gradient flow dynamics: ODE

$$\dot{x}(t) = -\nabla f(x(t))$$

$\dot{x}(t) \in X$ provides the **rate (or velocity)** (we can see)

$-\nabla f(x(t)) \in X^*$ provides the **(thermodynamic) force** (can't see; shadow price)

The equation should be written in the **force-balance** form

$$\mathbb{I}_R \dot{x}(t) = -\nabla f(x(t)) \in X^*, \quad \mathbb{I}_R : X \to X^* \text{ is the Riesz isomorphism.}$$

If $X \ncong X^*$: $\dot{u} \in \partial R^*(\mu, -\mathrm{D}F) \subset \mathrm{T}_u M$ (**rate**) **vs** $0 \in \mathrm{D}F + \partial R(\mu, \dot{\mu}) \subset \mathrm{T}^*_u M$ (**force**)

Duality in gradient flow dynamics: ODE

$$\dot{x}(t) = -\nabla f(x(t))$$

$\dot{x}(t) \in X$ provides the **rate (or velocity)** (we can see)

$-\nabla f(x(t)) \in X^*$ provides the **(thermodynamic) force** (can't see; shadow price)

The equation should be written in the **force-balance** form

$$\mathbb{I}_R \dot{x}(t) = -\nabla f(x(t)) \in X^*, \quad \mathbb{I}_R : X \to X^* \text{ is the Riesz isomorphism.}$$

If $X \ncong X^*$: $\dot{u} \in \partial R^*(\mu, -\mathrm{D}F) \subset \mathrm{T}_u M$ (**rate**) **vs** $0 \in \mathrm{D}F + \partial R(\mu, \dot{\mu}) \subset \mathrm{T}^*_u M$ (**force**)

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

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

Duality in gradient flow dynamics: ODE

$$\dot{x}(t) = -\nabla f(x(t))$$

$\dot{x}(t) \in X$ provides the **rate (or velocity)** (we can see)

$-\nabla f(x(t)) \in X^*$ provides the **(thermodynamic) force** (can't see; shadow price)

The equation should be written in the **force-balance** form

$$\mathbb{I}_R \dot{x}(t) = -\nabla f(x(t)) \in X^*, \quad \mathbb{I}_R : X \to X^* \text{ is the Riesz isomorphism.}$$

If $X \ncong X^*$: $\dot{u} \in \partial R^*(\mu, -\mathrm{D}F) \subset \mathrm{T}_u M$ (**rate**) **vs** $0 \in \mathrm{D}F + \partial R(\mu, \dot{\mu}) \subset \mathrm{T}_u^* M$ (**force**)

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

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

Duality in gradient flow dynamics: ODE

$$\dot{x}(t) = -\nabla f(x(t))$$

$\dot{x}(t) \in X$ provides the **rate (or velocity)** (we can see)

$-\nabla f(x(t)) \in X^*$ provides the **(thermodynamic) force** (can't see; shadow price)

The equation should be written in the **force-balance** form

$$\mathbb{I}_R \dot{x}(t) = -\nabla f(x(t)) \in X^*, \quad \mathbb{I}_R : X \to X^* \text{ is the Riesz isomorphism.}$$

If $X \ncong X^*$: $\dot{u} \in \partial R^*(\mu, -\mathrm{D}F) \subset \mathrm{T}_u M$ (**rate**) **vs** $0 \in \mathrm{D}F + \partial R(\mu, \dot{\mu}) \subset \mathrm{T}^*_u M$ (**force**)

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

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

Duality in gradient flow dynamics: ODE

$$\dot{x}(t) = -\nabla f(x(t))$$

$\dot{x}(t) \in X$ provides the **rate (or velocity)** (we can see)

$-\nabla f(x(t)) \in X^*$ provides the **(thermodynamic) force** (can't see; shadow price)

The equation should be written in the **force-balance** form

$$\mathbb{I}_R \dot{x}(t) = -\nabla f(x(t)) \in X^*, \quad \mathbb{I}_R : X \to X^* \text{ is the Riesz isomorphism.}$$

If $X \ncong X^*$: $\dot{u} \in \partial R^*(\mu, -\mathrm{D}F) \subset \mathrm{T}_u M$ (**rate**) **vs** $0 \in \mathrm{D}F + \partial R(\mu, \dot{\mu}) \subset \mathrm{T}^*_u M$ (**force**)

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

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

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

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

Duality in the Wasserstein gradient flow

Wasserstein gradient flow in the **rate** form (primal; vs. force-balance)

$$\partial_t \mu = -\mathbb{K}_{\mathsf{Otto}}(\mu)\ \mathrm{D}F$$

Duality in the Wasserstein gradient flow

Wasserstein gradient flow in the **rate** form (primal; vs. force-balance)

$$\partial_t \mu = -\mathbb{K}_{\mathsf{Otto}}(\mu)\ \mathrm{D}F = \nabla \cdot (\mu \nabla \mathrm{D}F).$$

Duality in the Wasserstein gradient flow

Wasserstein gradient flow in the **rate** form (primal; vs. force-balance)

$$\partial_t \mu = -\mathbb{K}_{\mathsf{Otto}}(\mu)\,\mathrm{D}F = \nabla \cdot (\mu \nabla \mathrm{D}F).$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t} F(\mu(t)) = -\frac{1}{2}|\mu'|_{W_2}(t)^2 - \frac{1}{2}|\nabla^- F|_{W_2}(\mu(t))^2$$

Duality in the Wasserstein gradient flow

Wasserstein gradient flow in the **rate** form (primal; vs. force-balance)

$$\partial_t \mu = -\mathbb{K}_{\mathsf{Otto}}(\mu)\ \mathrm{D}F = \nabla \cdot (\mu \nabla \mathrm{D}F).$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t} F(\mu(t)) = -\frac{1}{2}|\mu'|_{W_2}(t)^2 - \frac{1}{2}|\nabla^- F|_{W_2}(\mu(t))^2$$

For (Boltzmann) entropy $F(u) = \rho \log \rho$, the *metric slope* is

$$|\nabla^- F|_{W_2}(\mu(t))^2 = \int |\nabla \log \rho|^2 \rho \ \mathrm{d}x$$

Duality in the Wasserstein gradient flow

Wasserstein gradient flow in the **rate** form (primal; vs. force-balance)

$$\partial_t \mu = -\mathbb{K}_{\mathsf{Otto}}(\mu)\ \mathrm{D}F = \nabla \cdot (\mu \nabla \mathrm{D}F).$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t} F(\mu(t)) = -\frac{1}{2} |\mu'|_{W_2}(t)^2 - \frac{1}{2} |\nabla^- F|_{W_2}(\mu(t))^2$$

For (Boltzmann) entropy $F(u) = \rho \log \rho$, the *metric slope* is

$$|\nabla^- F|_{W_2}(\mu(t))^2 = \int |\nabla \log \rho|^2 \rho \ \mathrm{d}x$$

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

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

density $\rho := \frac{\mathrm{d}\mu}{\mathrm{d}\mathcal{L}}$ and force field $\frac{\delta F}{\delta \mu}[\mu]$ are **not accessible** if μ is atomic.

Kernel gradient flow as dual space force-balance

Motivated by the "Kernel DRO-type" derivation in [Zhu et al.'21, Kremer et al.'23],

Kernel gradient flow as dual space force-balance

Motivated by the "Kernel DRO-type" derivation in [Zhu et al.'21, Kremer et al.'23],

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**

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

where convolution $k * \mu := \int k(x, \cdot)\mu(\,\mathrm{d}x)$.

Kernel gradient flow as dual space force-balance

Motivated by the "Kernel DRO-type" derivation in [Zhu et al.'21, Kremer et al.'23],

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**

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

where convolution $k * \mu := \int k(x, \cdot)\mu(\,\mathrm{d}x)$. If F is entropy, ∇g "matches the score" .

Kernel gradient flow as dual space force-balance

Motivated by the "Kernel DRO-type" derivation in [Zhu et al.'21, Kremer et al.'23],

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**

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

where convolution $k * \mu := \int k(x, \cdot)\mu(\,\mathrm{d}x)$. If F is entropy, ∇g "matches the score" .

Compared with the Wasserstein GF of entropy, our kernel geometry 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, we have a **"dynamic formulation" of the dual DRO problem** [Zhu et al. 2021]

$$\min_{\theta} \sup_{\mathrm{MMD}(P,\hat{P})\le\epsilon} \mathbb{E}_P\, l(\theta,\xi),$$

Back to (kernel) robust learning

Motivated by our insight so far, we have a **"dynamic formulation" of the dual DRO** problem [Zhu et al. 2021]

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

the distribution shift (a.k.a. adversarial attack) is modeled by the dynamical system of the dual force-balance kernel gradient flow

$$k * \dot{\mu} = -g, \quad \mu(0) = \hat{P}, \mu(T) = P.$$

where $\nabla g(x)$ approximates the gradient $\nabla l(\theta, \xi)$.

Back to (kernel) robust learning

Motivated by our insight so far, we have a **“dynamic formulation” of the dual DRO** problem [Zhu et al. 2021]

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

the distribution shift (a.k.a. adversarial attack) is modeled by the dynamical system of the dual force-balance kernel gradient flow

$$k * \dot{\mu} = -g, \quad \mu(0) = \hat{P}, \mu(T) = P.$$

where $\nabla g(x)$ approximates the gradient $\nabla l(\theta,\xi)$.

Implication: a **general-purpose measure optimization algorithm operated in the dual space** (see also the preprint on kernel mirror prox. [Dvurechensky & Zhu])

Summary

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):
  - force vs. rate

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):
  - force vs. rate
- Role of the **dual kernel function** in this talk

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):
  - force vs. rate
- Role of the **dual kernel function** in this talk
  - **robust surrogate loss** (flatten the curve)

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):
  - force vs. rate
- Role of the **dual kernel function** in this talk
  - **robust surrogate loss** (flatten the curve)
  - **optimal test fcn. for two-sample test**

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):
  - force vs. rate
- Role of the **dual kernel function** in this talk
  - **robust surrogate loss** (flatten the curve)
  - **optimal test fcn. for two-sample test**
  - **approximate force field**

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):
  - force vs. rate
- Role of the **dual kernel function** in this talk
  - **robust surrogate loss** (flatten the curve)
  - **optimal test fcn. for two-sample test**
  - **approximate force field**
- Our kernel scheme (DRO, GF) is designed to treat

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):
  - force vs. rate
- Role of the **dual kernel function** in this talk
  - **robust surrogate loss** (flatten the curve)
  - **optimal test fcn. for two-sample test**
  - **approximate force field**
- Our kernel scheme (DRO, GF) is designed to treat
  - Energy that's the **integral of nonlinear functions** or **nonlinear in measures**
    $$F(\mu) = \int V \,\mathrm{d}\mu, \qquad F(\mu) = \int \phi(\rho) \quad (\mu = \rho \cdot \mathscr{L})$$
    which are challenging for computation using the WGF (complication due to W-geodesics).

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):
  - force vs. rate
- Role of the **dual kernel function** in this talk
  - **robust surrogate loss** (flatten the curve)
  - **optimal test fcn. for two-sample test**
  - **approximate force field**
- Our kernel scheme (DRO, GF) is designed to treat
  - Energy that's the **integral of nonlinear functions** or **nonlinear in measures**
    $$F(\mu) = \int V \, \mathrm{d}\mu, \qquad F(\mu) = \int \phi(\rho) \quad (\mu = \rho \cdot \mathscr{L})$$
    which are challenging for computation using the WGF (complication due to W-geodesics).
- Other important uses of the dual kernel function: Causal inference, conditional moments, (robust) control and RL

Summary

- Two types of duality: **static** (DRO) to **dynamic** (GF):
  - force vs. rate
- Role of the **dual kernel function** in this talk
  - **robust surrogate loss** (flatten the curve)
  - **optimal test fcn. for two-sample test**
  - **approximate force field**
- Our kernel scheme (DRO, GF) is designed to treat
  - Energy that's the **integral of nonlinear functions** or **nonlinear in measures**

    $$F(\mu) = \int V \,\mathrm{d}\mu, \qquad F(\mu) = \int \phi(\rho) \qquad (\mu = \rho \cdot \mathscr{L})$$

    which are challenging for computation using the WGF (complication due to W-geodesics).
- Other important uses of the dual kernel function: Causal inference, conditional moments, (robust) control and RL

References:

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. Preprint

Download the slides:

Website: jj-zhu.github.io