From Gradient Flow Force-Balance to Distributionally Robust Learning

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Angewandte Analysis und Stochastik

Distributional robustness, but what kind?

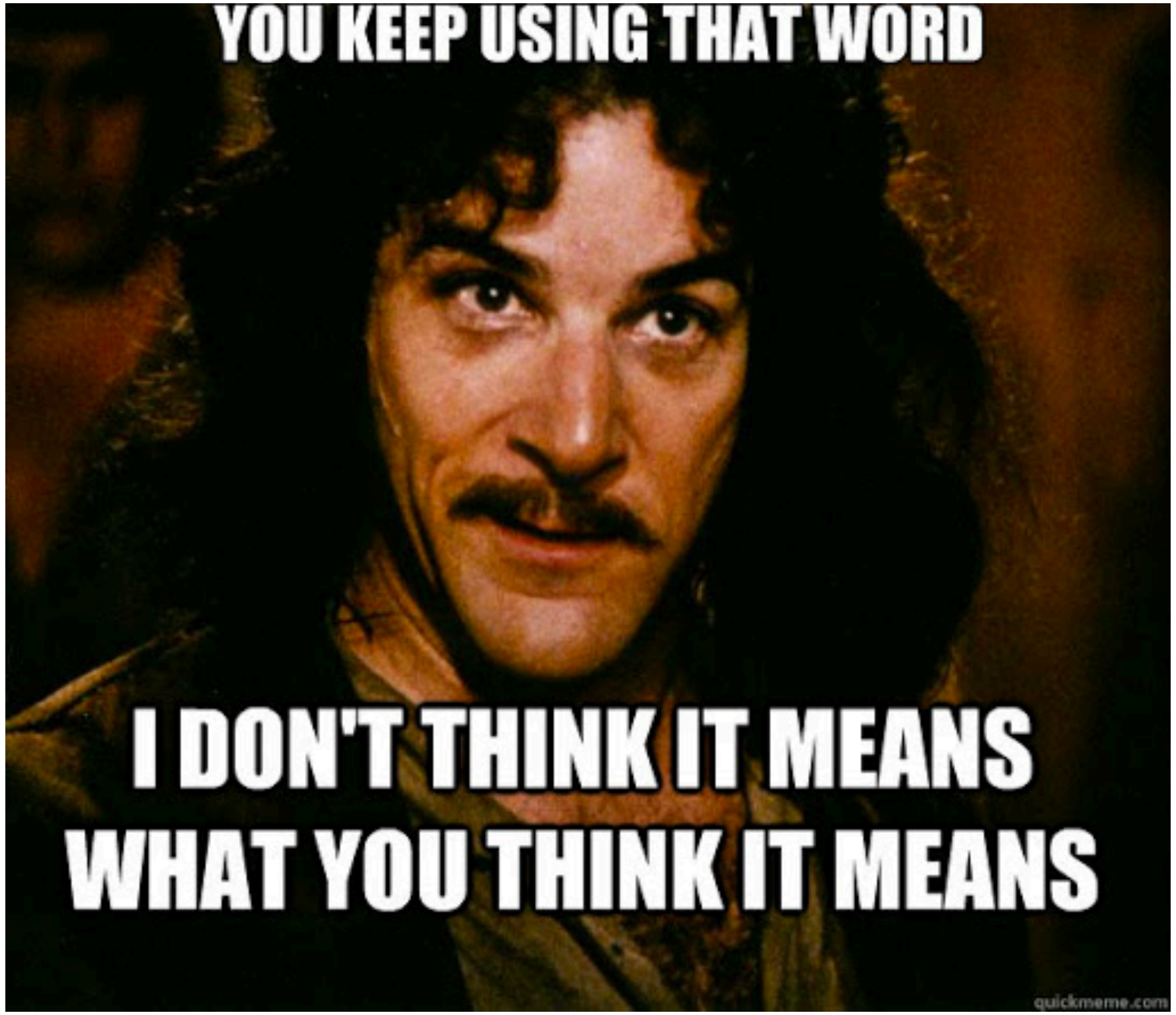


Figure credit: The Princess Bride,
a bedside story by your grandpa

Motivation: From statistical learning to 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 $(\neq P_0)$

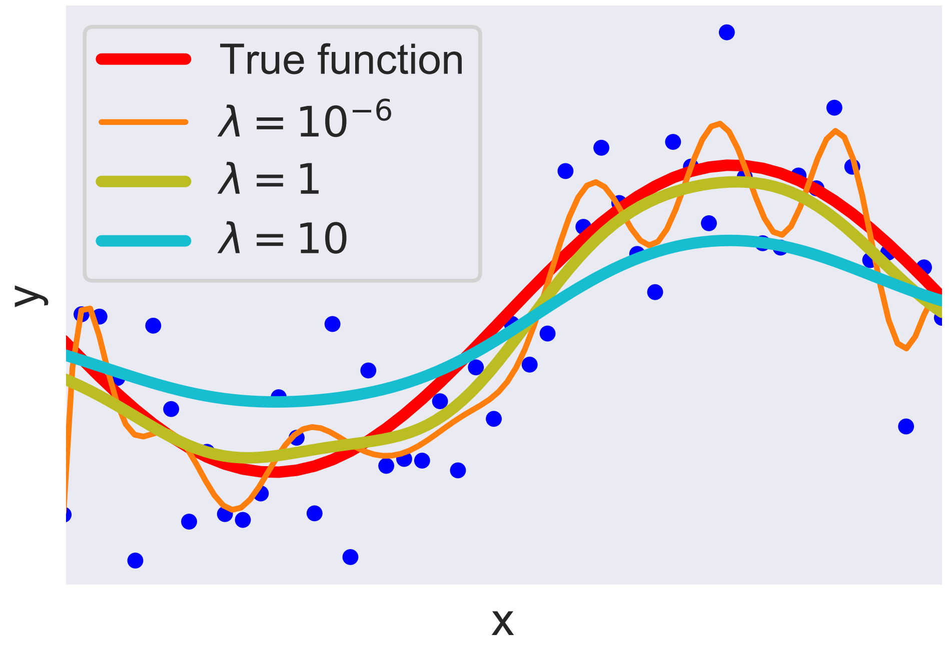
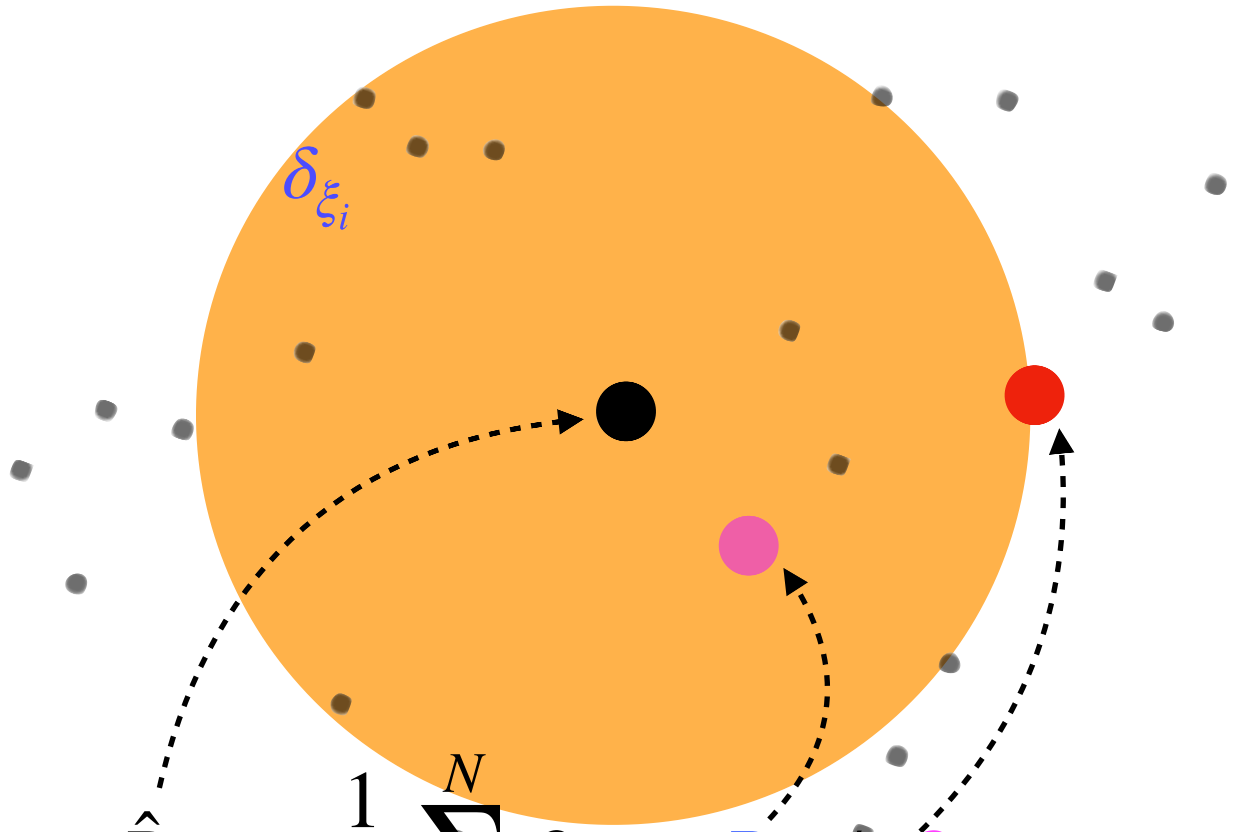


Figure credit: H. Kremer, J. Zhu

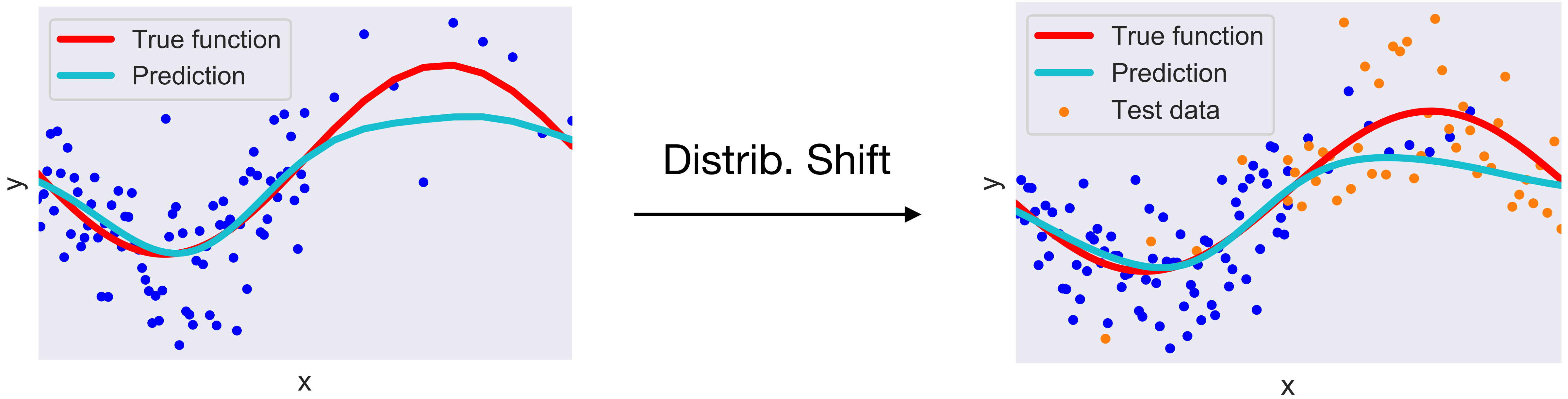


$$\hat{P}_N := \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_i} \Rightarrow P_0 \neq Q$$

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:

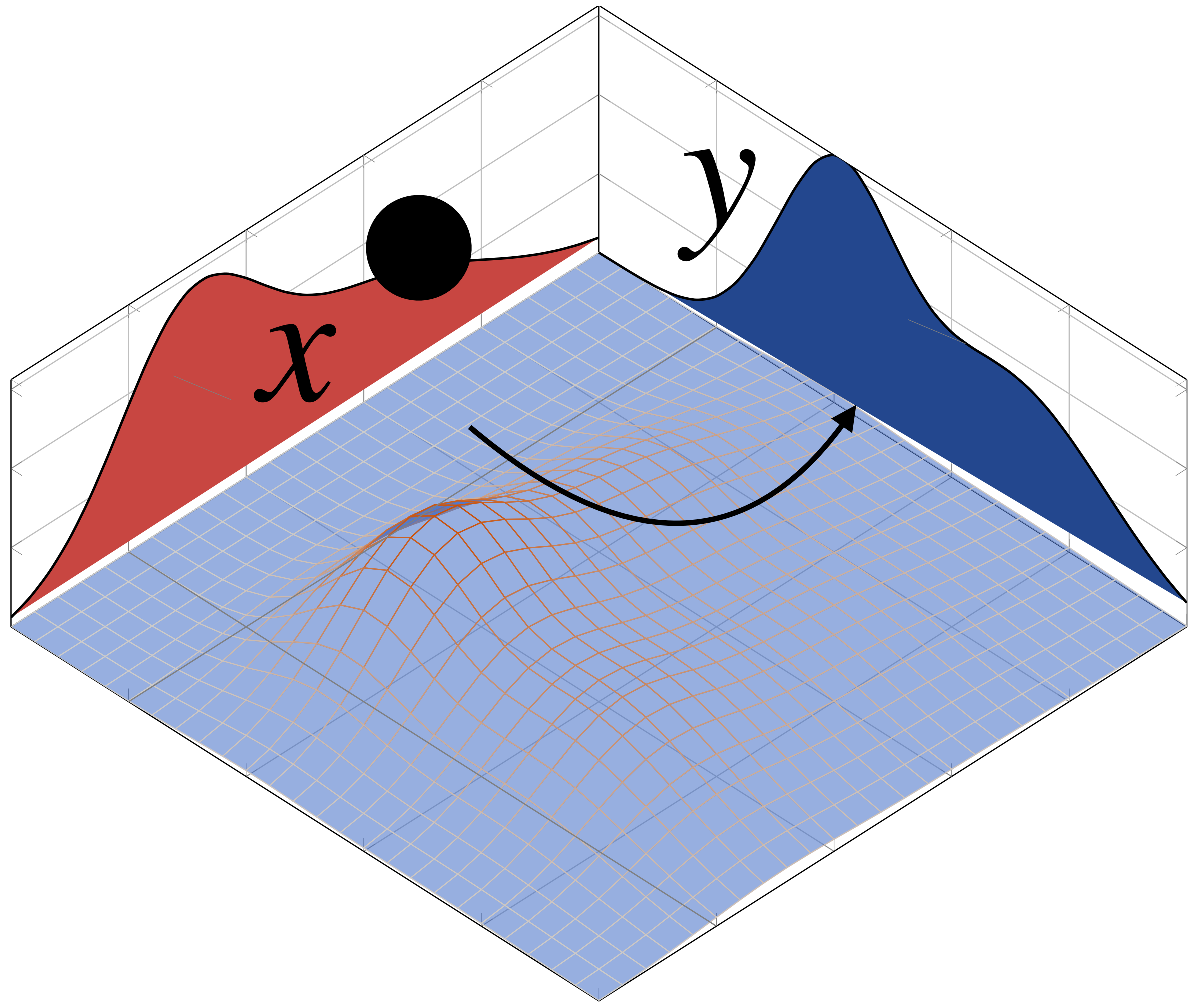
Information geometry [S. Amari et al.] e.g. descent in Fisher-Rao geometry

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

Background: Kantorovich-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: ***à la Benamou-Brenier***

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

Background: MMD and interaction force

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.

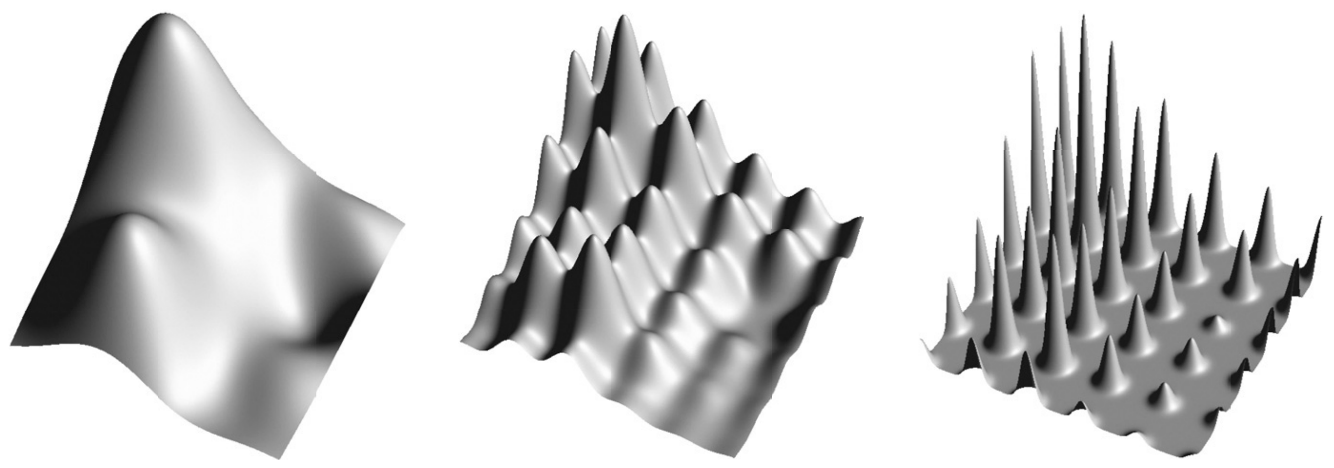
Dual formulation as an integral probability metric.

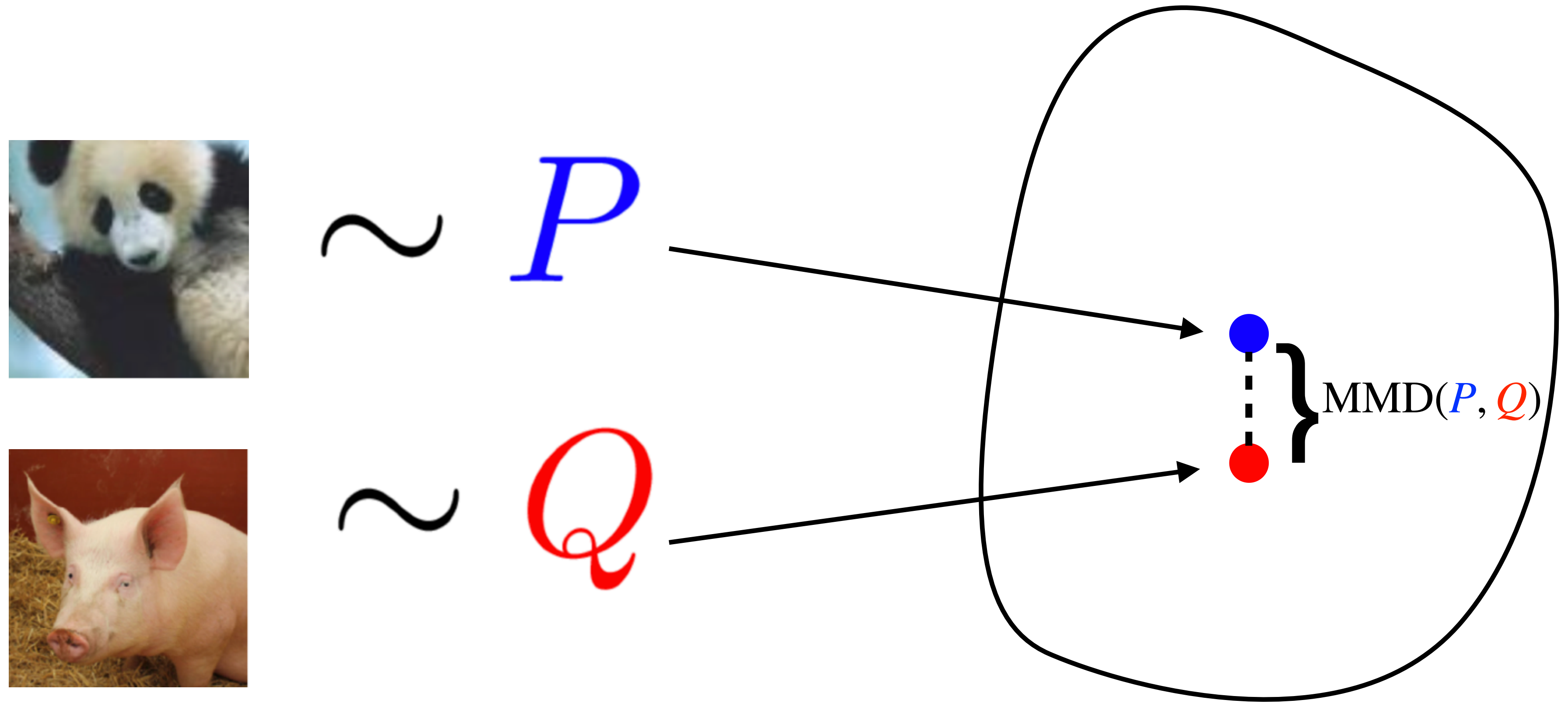
$$\mathrm{MMD}(P, Q) = \sup_{\|f\|_{\mathcal{H}} \leq 1} \int f \, d(P - Q)$$

$\mathcal{H}$ 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 $\mathcal{H}$.

As an interaction energy for Wasserstein GF [Arbel et al.]

$$\mathrm{MMD}^2(P, Q) = \iint k(x, y) \ \mathrm{d}(P - Q)(x) \ \mathrm{d}(P - Q)(y)$$





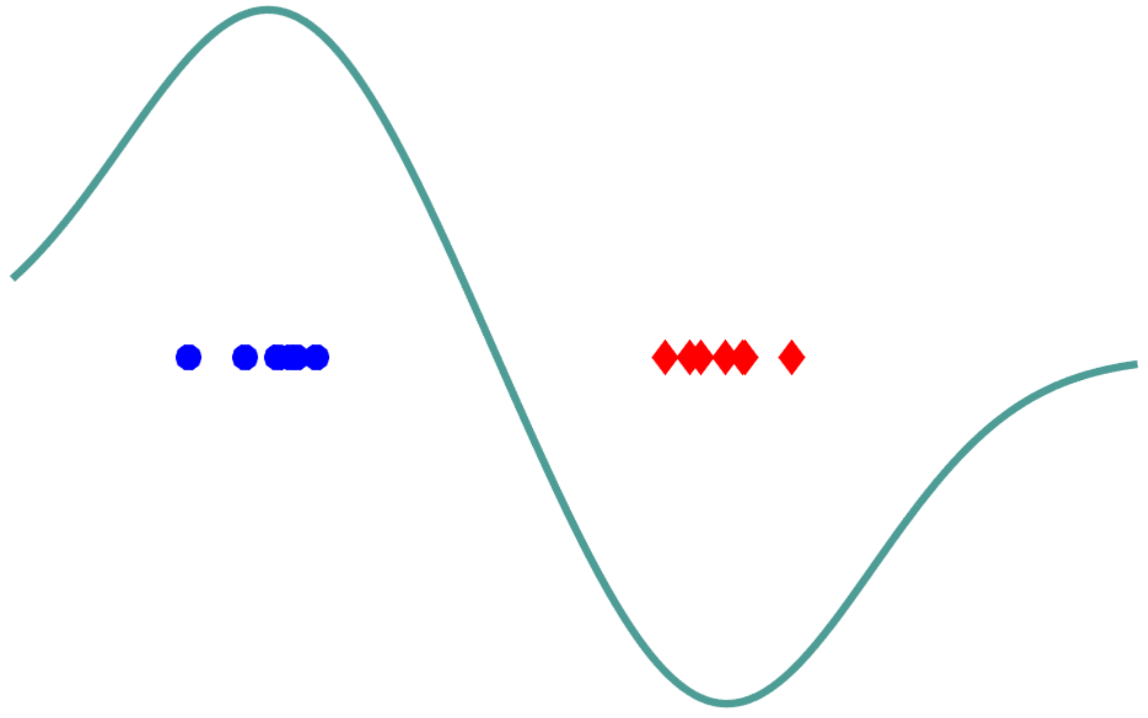


Figure credit: W. Jitkrittum, J. Zhu, H. Wendland

Gradient Flow Force-Balance

Gradient flow facts

Otto's Gradient flow equation in the Wasserstein space

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

e.g., diffusion, Fokker Planck equation. It describes the "steepest" dissipation of energy F in $(\mathrm{Prob}(\bar{X}), W_2)$. [Otto et al 2000s, Ambrosio 2005, ...]

In a different flavor, we can write it just like ODE gradient flow $\dot{x} = -\nabla f(x)$ in the **primal rate-form**

$$\dot{\mu} = -\mathbb{K}_{\text{Otto}}(\mu)\ \mathrm{D}F$$ ($\mathrm{D}F$ is the (sub)diff., e.g., in the sense of Fréchet)

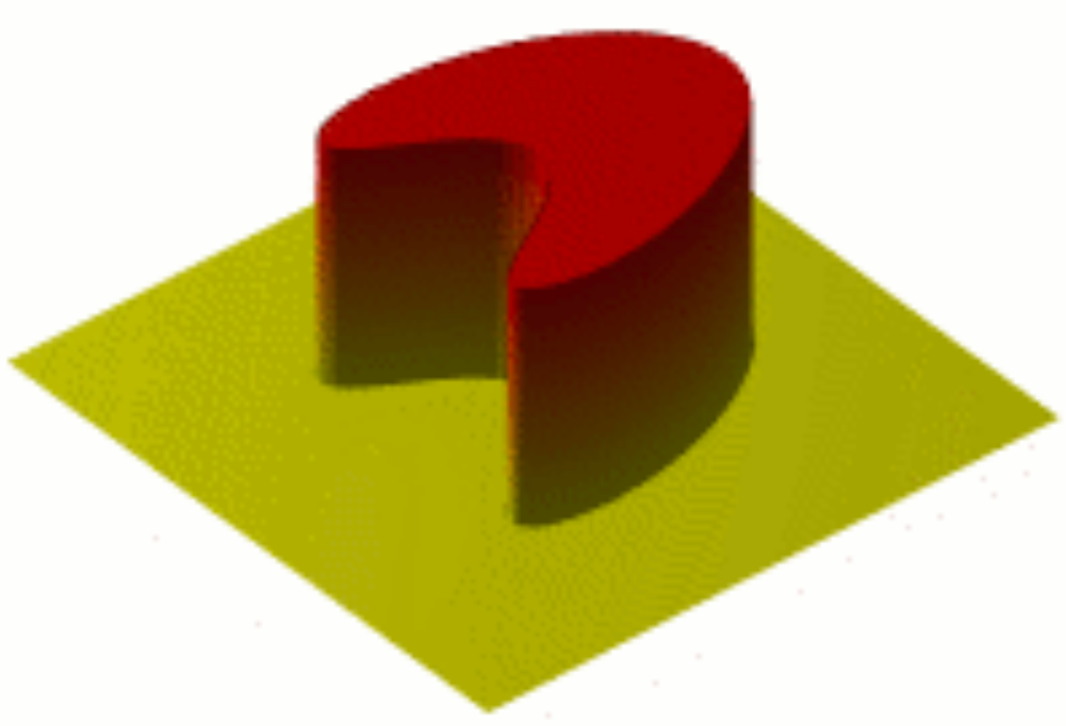
Time-discretization yields the *minimizing movement scheme* (MMS)

"JKO Scheme" $$u_k \in \arg\inf_{u \in \mathscr{P}} F(u) + \frac{1}{2\tau} W_2^2\left(u, u_{k-1}\right)$$

SIAM J. MATH. ANAL.
Vol. 29, No. 1, pp. 1–17, January 1998

THE VARIATIONAL FORMULATION OF THE FOKKER–PLANCK EQUATION*

RICHARD JORDAN†, DAVID KINDERLEHRER‡, AND FELIX OTTO§

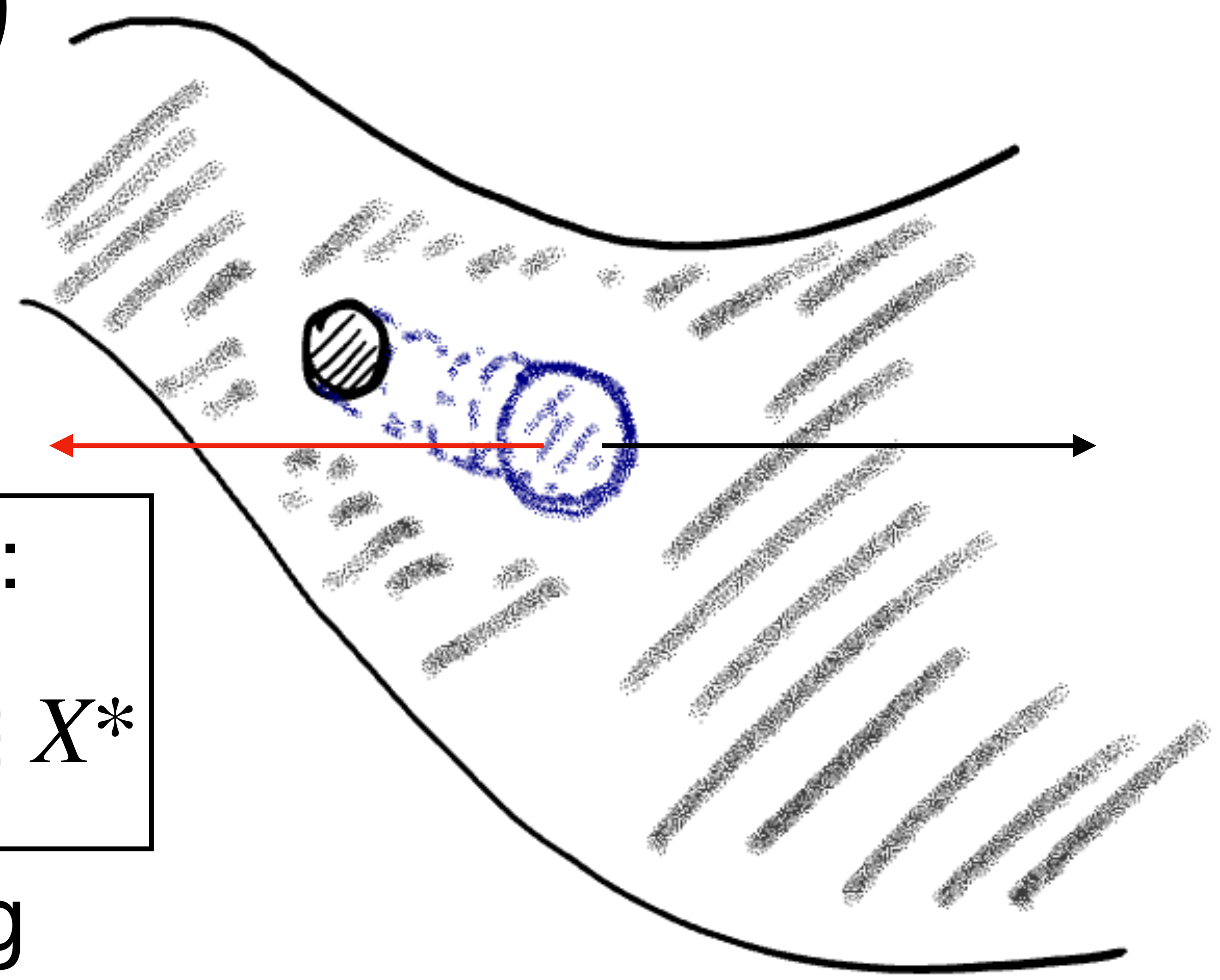


ODE flow: gradient descent

$$x^k \in \arg\min_{x \in \mathbb{R}^d} F(x) + \frac{1}{2\tau}\|x - x^{k-1}\|^2.$$

Gradient flow force-balance

Force-balance in Wasserstein MMS $u_k \in \arg\inf_{u\in\mathscr{P}} \; F(u) + \frac{1}{2\tau} W_2^2\left(u, u_{k-1}\right)$



$$\mathrm{D}F + \frac{\phi}{\tau} = \text{const}\,.\,,\ \phi : \text{“Kantorovich potential”}$$

Force:
drive movement
e.g., entropy

Dissipation Geometry:
resist movement
e.g., viscosity

Force-balance in ODE:

$$\nabla f(x_t) + \frac{x_t^\top - x_{t-1}^\top}{\tau} = 0 \in X^*$$

In practice, approximate ϕ (and hence $-\mathrm{D}F$) based on data samples using **function approximators** (force matching, score matching), NN/RKHS, e.g.,

$$\phi \approx f = \sum_{i=1}^{n} \alpha_i k(x_i, \cdot\,) \in \mathscr{H}\,.$$

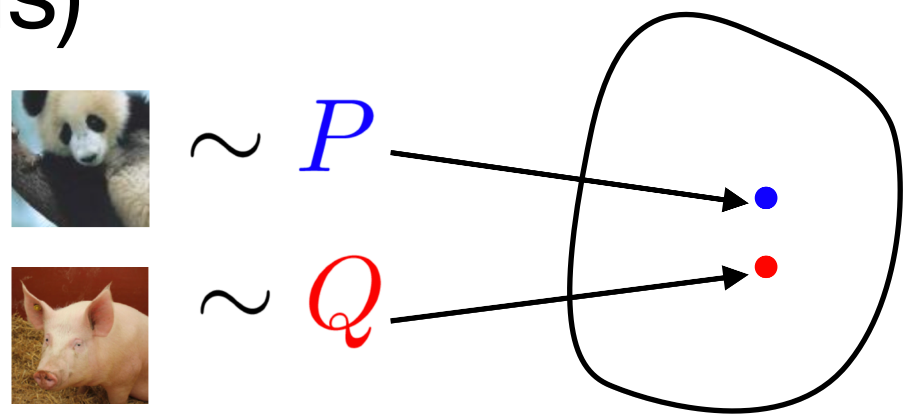
We will now see two applications of this force-balance relation to robust learning

Robust Learning under (Joint) Distribution Shift

Kernel DRO under distribution shift

Primal DRO (not solvable as it is)

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

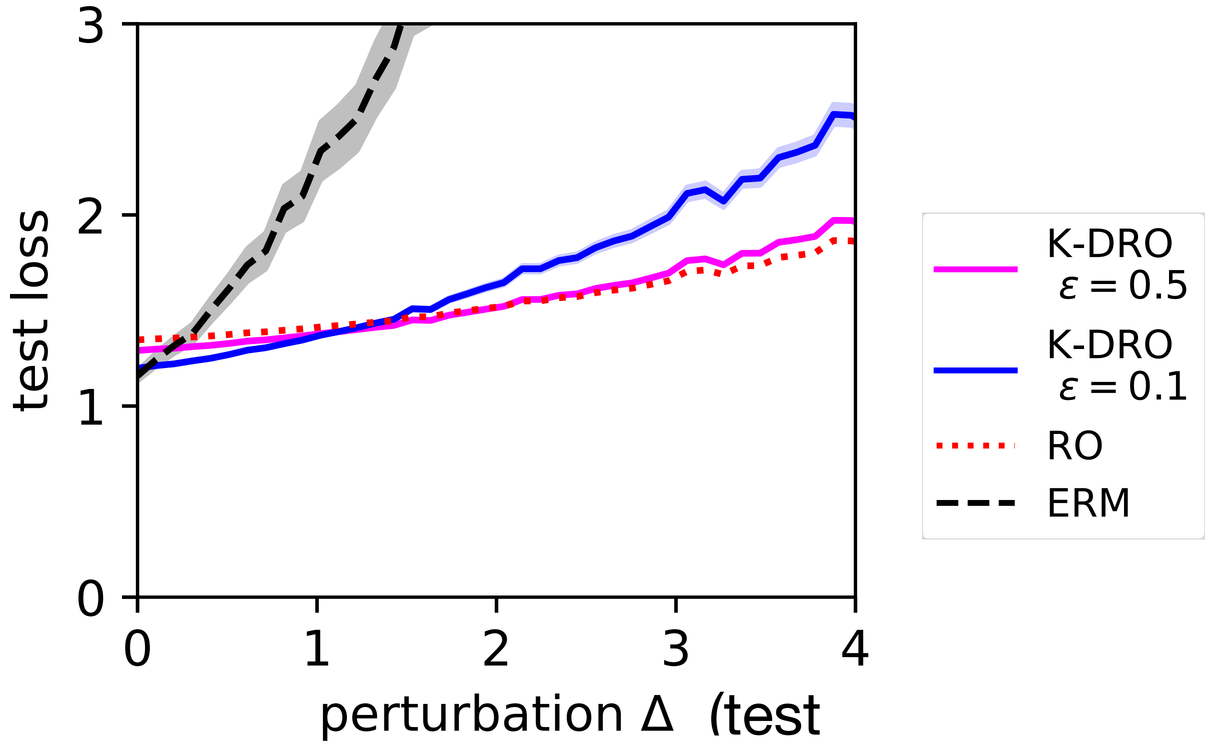


Kernel DRO Theorem (simplified). [Z. et al. 2021]
DRO problem is equivalent to the dual kernel machine learning problem, i.e., (DRO)=(K).

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

Example. Robust least squares

$$\min \; l(\theta,\xi) := \|A(\xi)\cdot\theta - b\|_2^2$$



Entropy regularization ("interior point method")

$$\mathrm{MMD}(Q,\hat{P}) + \lambda D_{\phi}(Q\|\omega) \le \epsilon$$

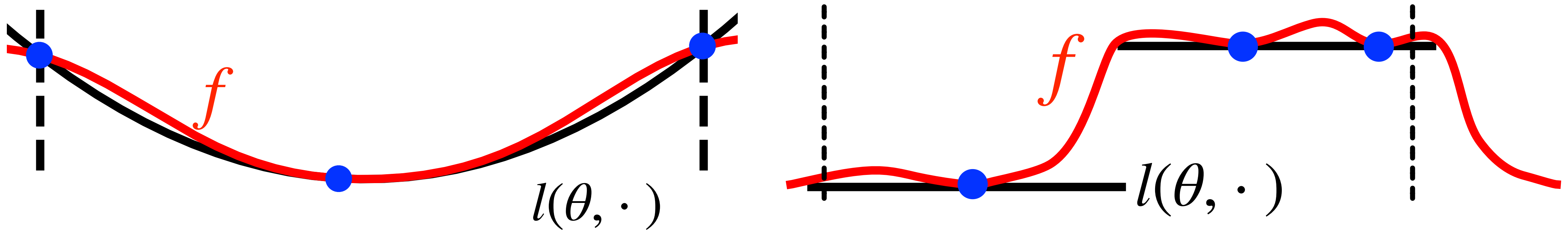
Dual. Adapted from [Kremer et al., **Z.** 2023]

$$\inf_{\theta, f\in\mathcal{H}} \left\{ \mathbb{E}_{\hat{P}} f + \epsilon\|f\|_{\mathcal{H}} + \lambda \mathbb{E}_{\omega}\phi^*\left(\frac{-f+l}{\lambda}\right)\right\}$$

soft cons. $\phi^*_{\mathrm{KL}}(t) = \exp(t)$

log-barrier $\phi^*_{\log}(t) = -\log(1-t)$

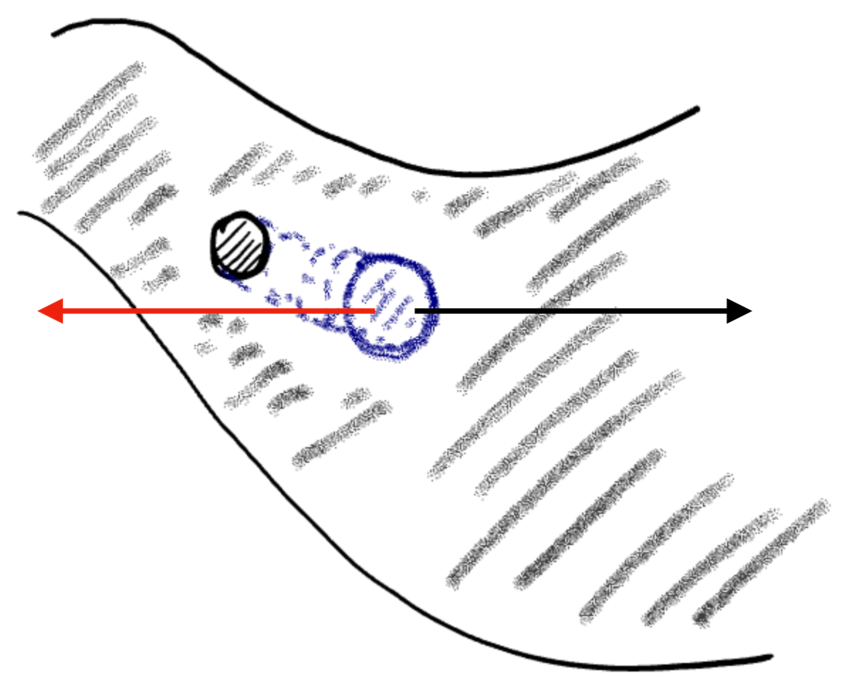
Geometric intuition: **dual kernel function f** as robust surrogate losses (flatten the curve)



Force-balance of Kernel DRO

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

Lagrangian: $\min_{\theta,\gamma\ge 0} \boxed{\sup_{\mu\in\mathcal{P}} \mathbb{E}_\mu l(\theta,x) - \gamma\cdot \mathrm{MMD}^2(\mu,\hat{\mu}_N)} + \gamma\epsilon^2$



MMS in kernel-MMD

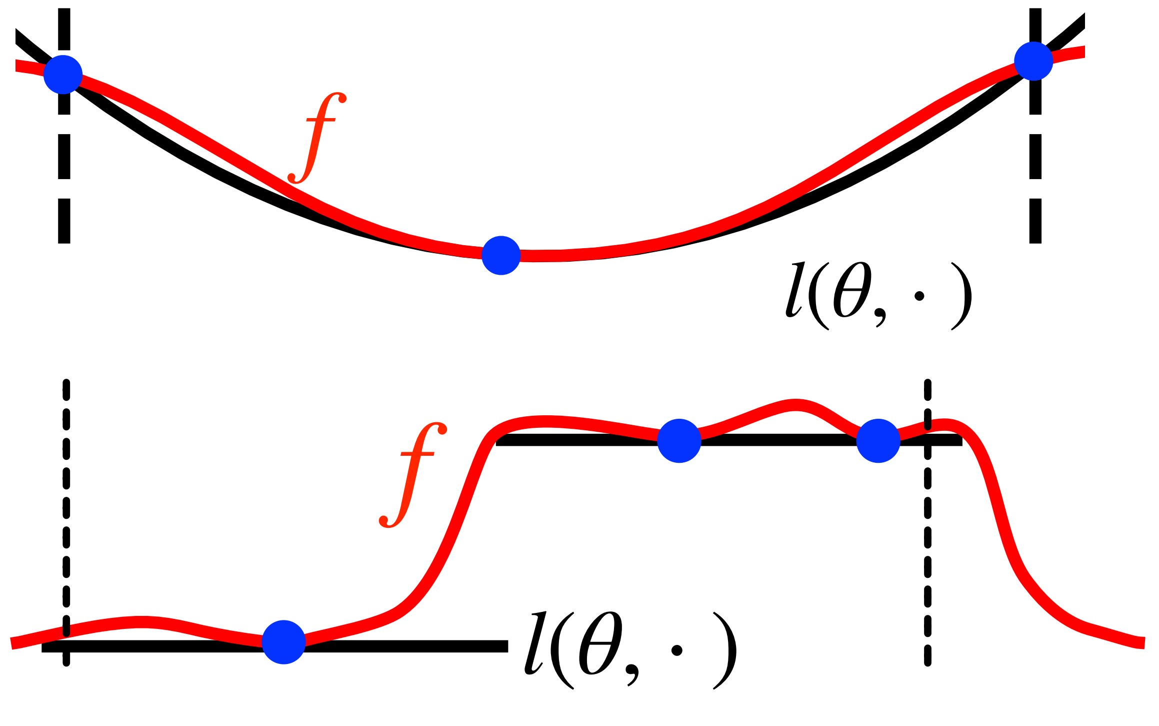
$$\inf_{\mu\in\mathcal{P}} F(\mu) + \frac{1}{2\tau}\mathrm{MMD}^2(\mu,\mu^k) \implies -\mathrm{D}^{L^2}F = \underbrace{\boxed{\frac{1}{\tau}\int k(x,\cdot)\mathrm{d}(\mu-\mu^k)(x)}}_{=:\, f\in\mathcal{H}} + \mathrm{const}$$

Dual kernel function f as robust surrogate losses

flatten the curve → force balance

Force-balance using **function approximation** RKHS functions, e.g.,

$$-\mathrm{D}F = f + f_0,\ f = \sum_{i=1}^{n} \alpha_i k(x_i,\cdot) \in \mathcal{H},\ f_0\in\mathbb{R}$$



$\mathrm{D}^{L^2}F = l(\theta,\cdot) \implies$ force-balance relation: $l(\theta,\cdot) = f + f_0$ a.e.

(force matching, score matching)

Robust Learning under Structured Distribution Shift

From statistical fluctuation to structured distribution shift

(Mild) (Strong)

Learning task
What can go wrong?

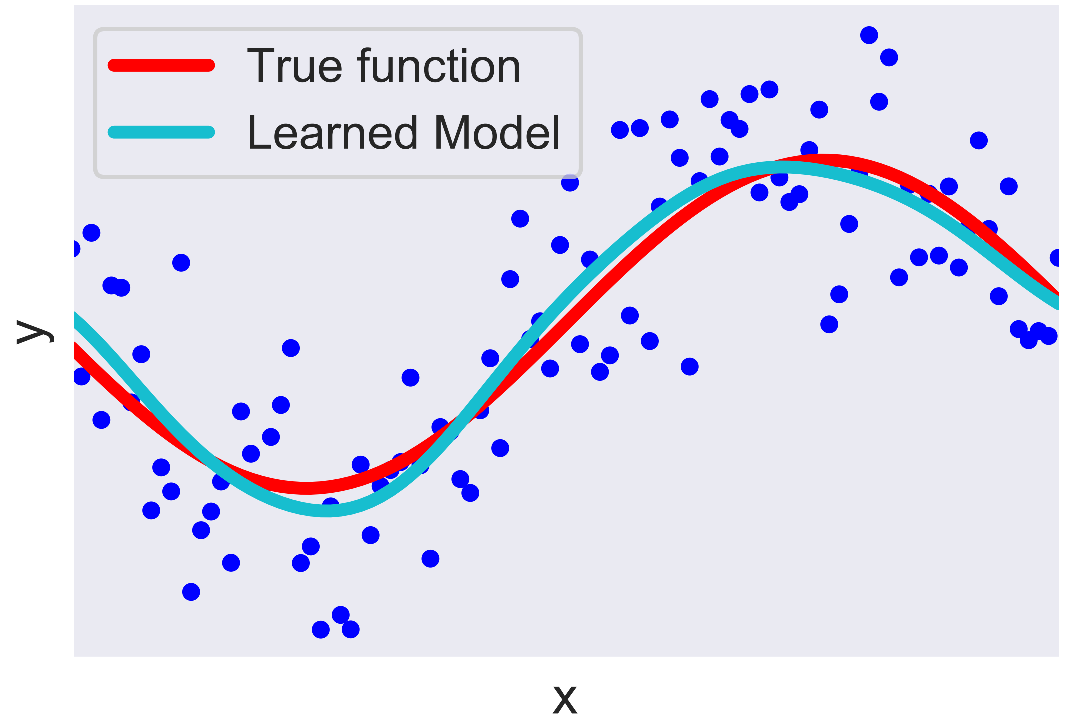
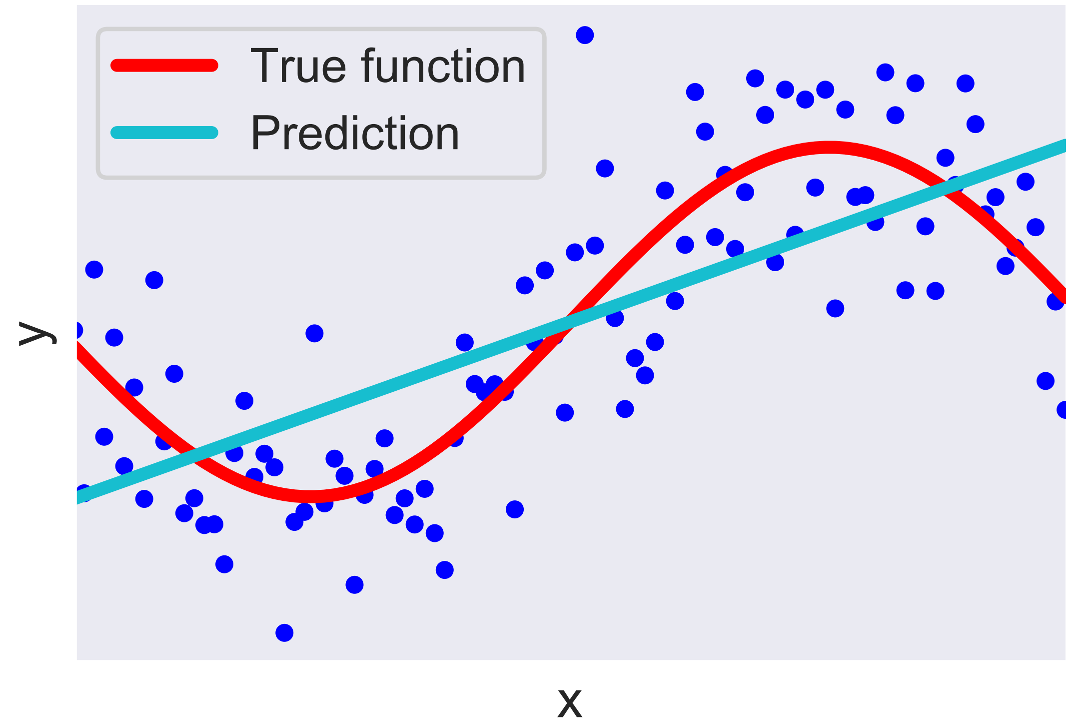


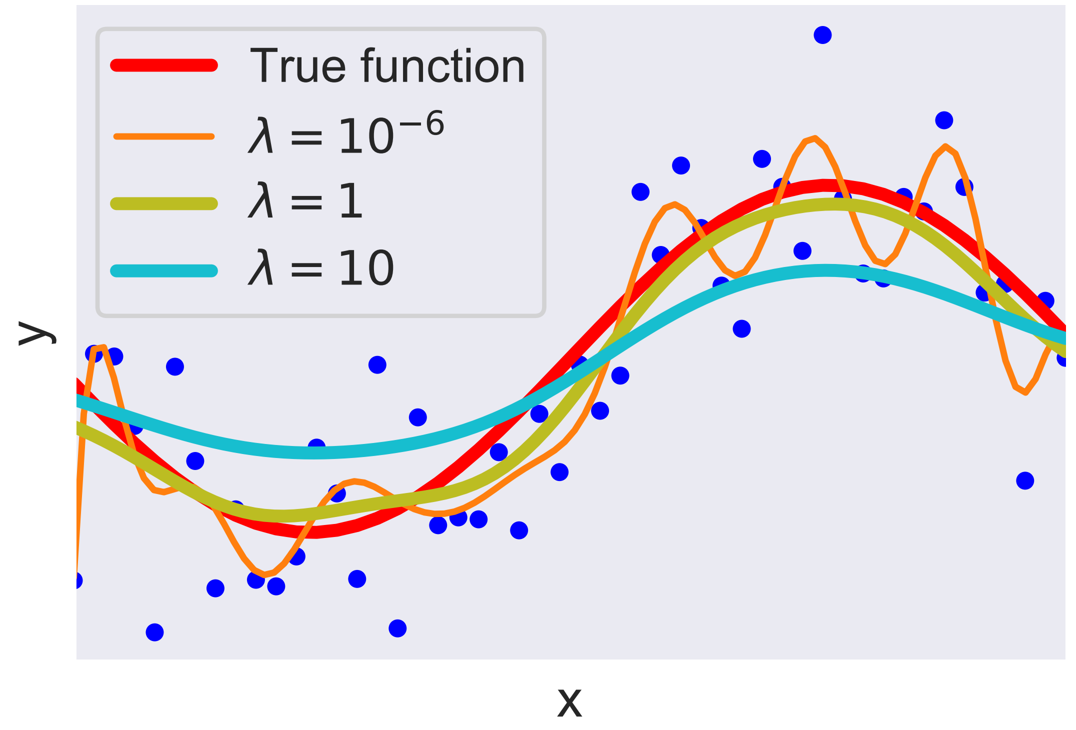
Figure credit: Heiner Kremer

Model mis-specification
$f_\theta \neq f \;\forall \theta \in \Theta$



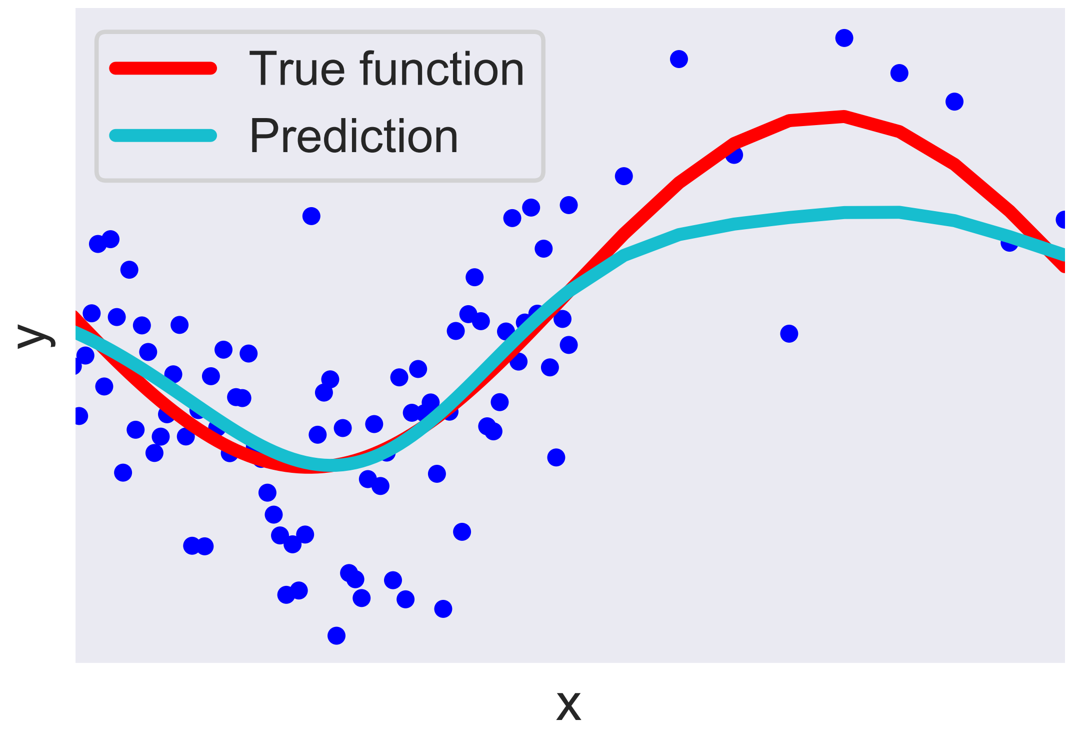
$\rightarrow$ Use flexible models (NN/non-parametric)

Finite sample bias
$n \ll \infty$



$\rightarrow$ Statistical learning theory/regularization

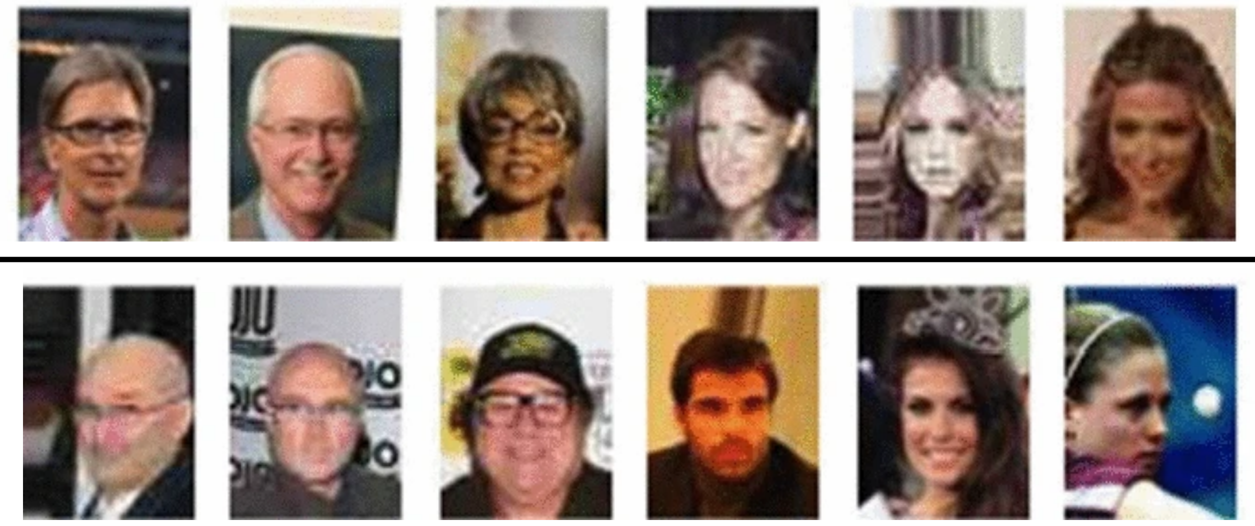
Distribution shifts
$\mathbb{P}_{\text{test}} \neq \mathbb{P}_{\text{train}}$



$\rightarrow$ Robustness, Causality

Q_{test}

$\hat{P}_{\text{train}}$



[Heinze-Deml & Meinshausen 2021]

waterbird + land

landbird + land

waterbird + water

[Sagawa et al. 2020]

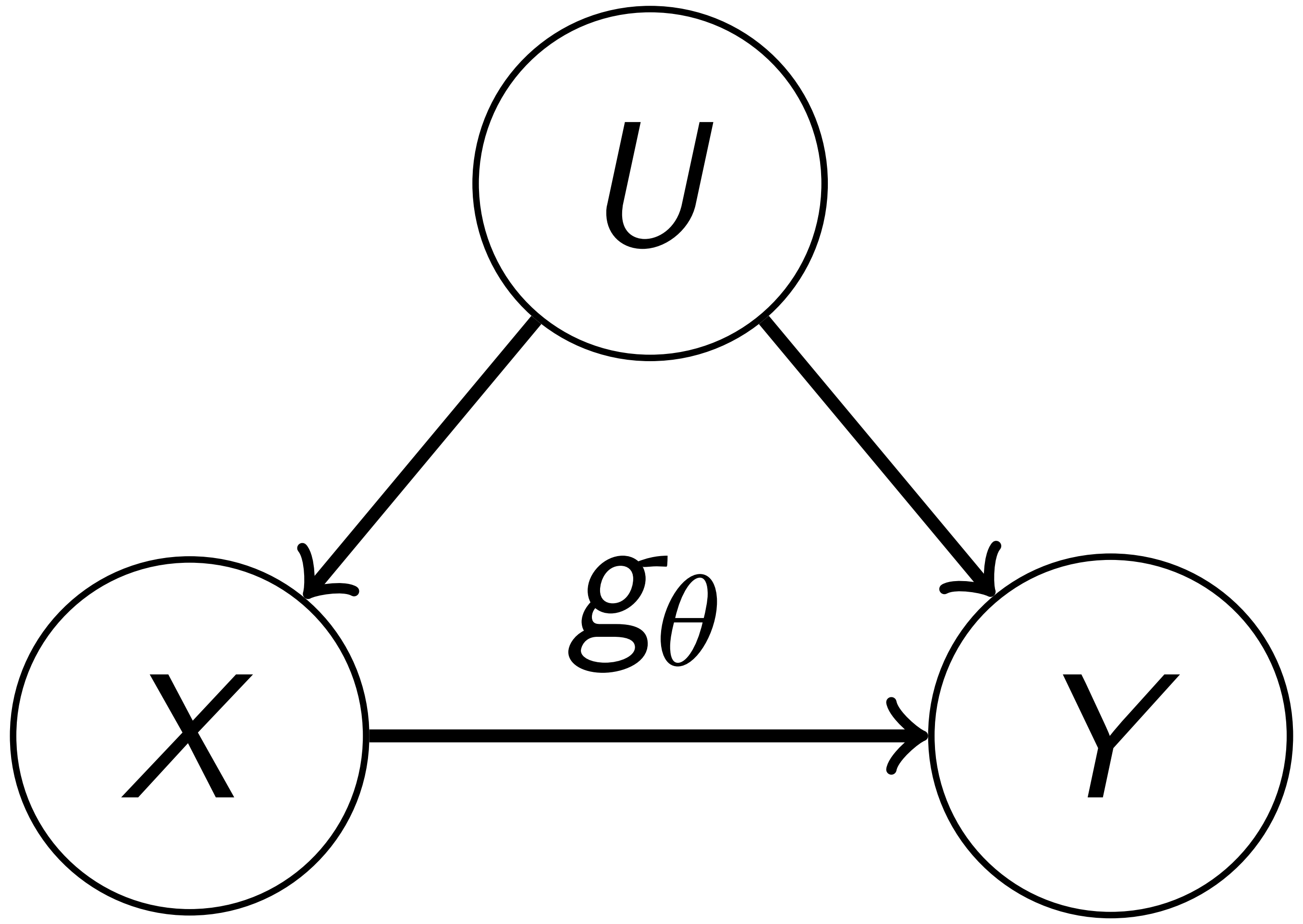
Wasserstein/Kernel DRO not suitable for (strong) structured distribution shifts !

Structured Distribution Shift — Causal Confounding

Causal confounding can lead to much **stronger** distribution shifts than those considered in (**joint**) distribution shift, e.g., DRO, adversarial robustness.

X: Smoking, Y: Cancer, U: Lifestyle

$$Y := g_\theta(X) + \epsilon_U, \quad \mathbb{E}[\epsilon_U] = 0, \text{ but } \mathbb{E}[\epsilon_U | X] \neq 0$$
$$\implies \quad g_\theta(x) \neq \mathbb{E}[Y | X = x]$$

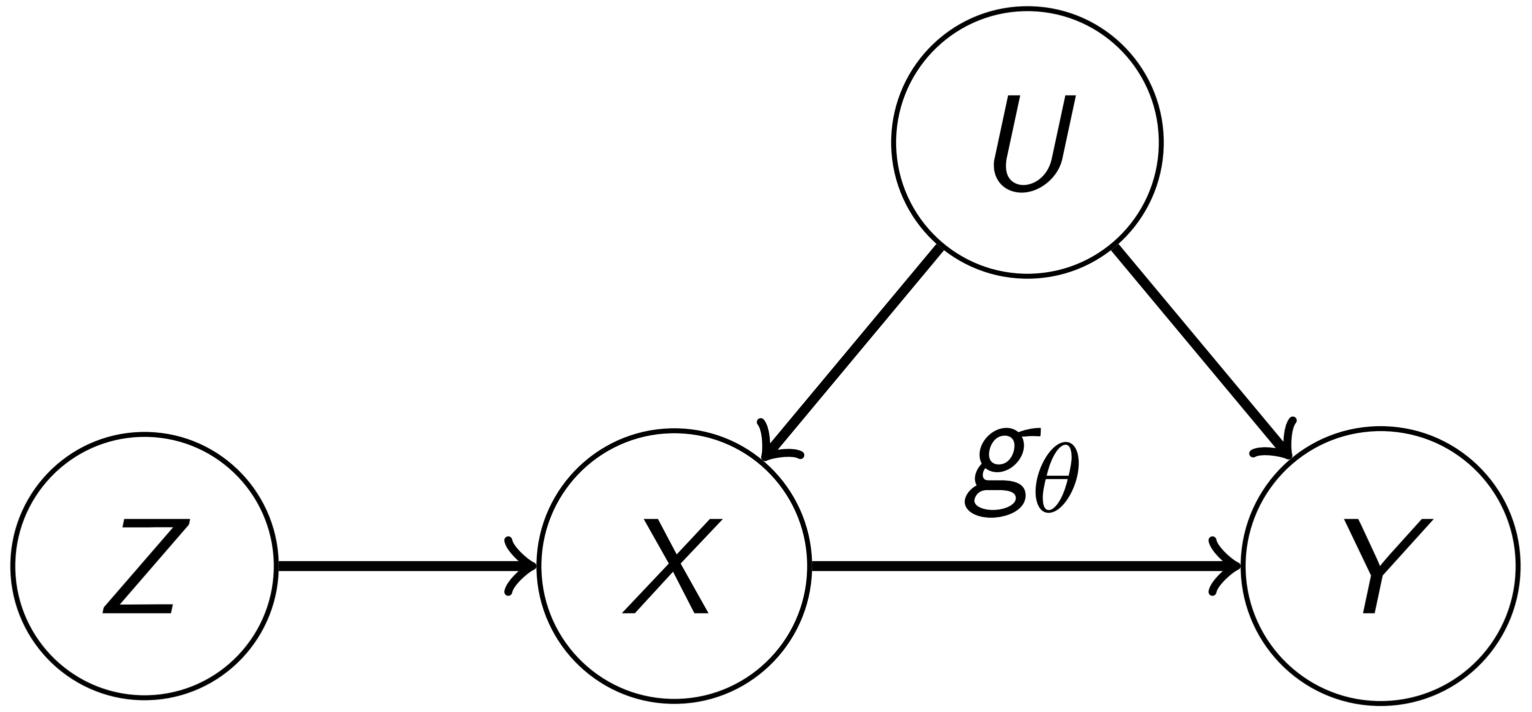


Regression $\min_\theta \mathbb{E}[\|Y - g_\theta(X)\|^2]$ or DRO does not work in this case.

Kernel Method of Moment: conditional moment restriction for causal inference

Robustness against **structured distribution shifts** instead of (joint-)DRO. Estimating g_θ via **conditional moment restriction (CMR)**

$$\mathbb{E}[Y - g_\theta(X) \,|\, Z] = 0 \ \mathbb{P}_Z\text{-a.s.}$$



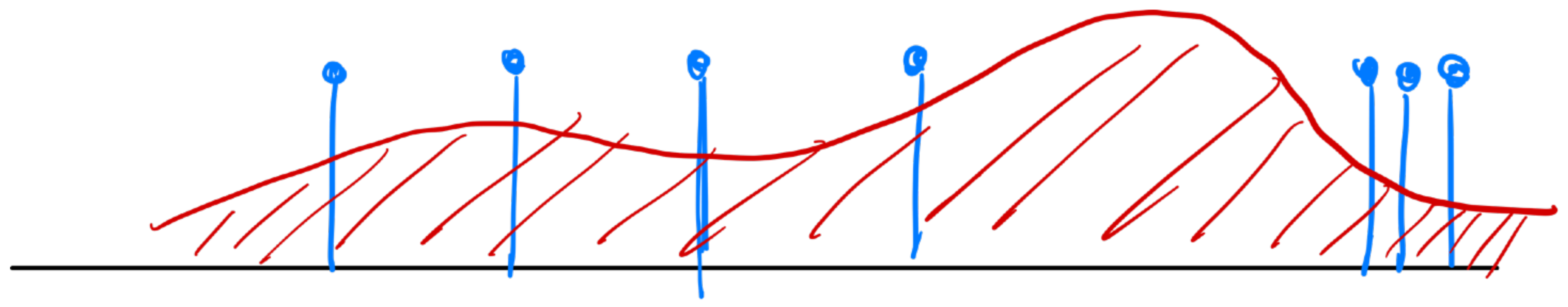
Instrument: Genetic predisposition for nicotine addiction Z

Generalized Empirical likelihood [Owen, 1988; Qin and Lawless, 1994] with **CMR** [Bierens, 1982]. Equivalently, generalized method of moment (GMM)

$$\inf_{\theta, Q \in \mathscr{P}} D_\phi(Q \| \hat{P}) \ \text{ s.t. } \ \mathbb{E}_Q\left[\left(Y - g_\theta(X)\right)^T h(Z)\right] = 0, \ \forall h \in \mathscr{H}$$

Kernel MoM [Kremer et al., **Z.** 2023] with CMR

$$\inf_{\theta, Q \in \mathscr{P}} \frac{1}{2} \mathrm{MMD}^2(Q, \hat{P}) \ \text{ s.t. } \ \mathbb{E}_Q\left[\left(Y - g_\theta(X)\right)^T h(Z)\right] = 0$$



Lift the restriction that Q is an atomic distribution

Kernel MoM: duality and algorithm

$$\theta^{\text{KMM}} = \arg\min_{\theta} R(\theta)$$

$$R(\theta) := \inf_{Q \in \mathscr{P}} \frac{1}{2} \text{MMD}^2(Q, \hat{P}) \;\; \text{s.t.} \;\; \mathbb{E}_Q \left[\left(\psi(X;\theta)\right)^T h(Z) \right] = 0$$

Theorem. [Kremer et al., Z. 2023] The MMD profile $R(\theta)$ has the strongly dual form

$$R(\theta) = \sup_{\substack{f_0 \in \mathbb{R}, f \in \mathscr{F}, \\ h \in \mathscr{H}}} f_0 + \frac{1}{n} \sum_{i=1}^{n} f(x_i, z_i) - \frac{1}{2} \|f\|_{\mathscr{F}}^2$$

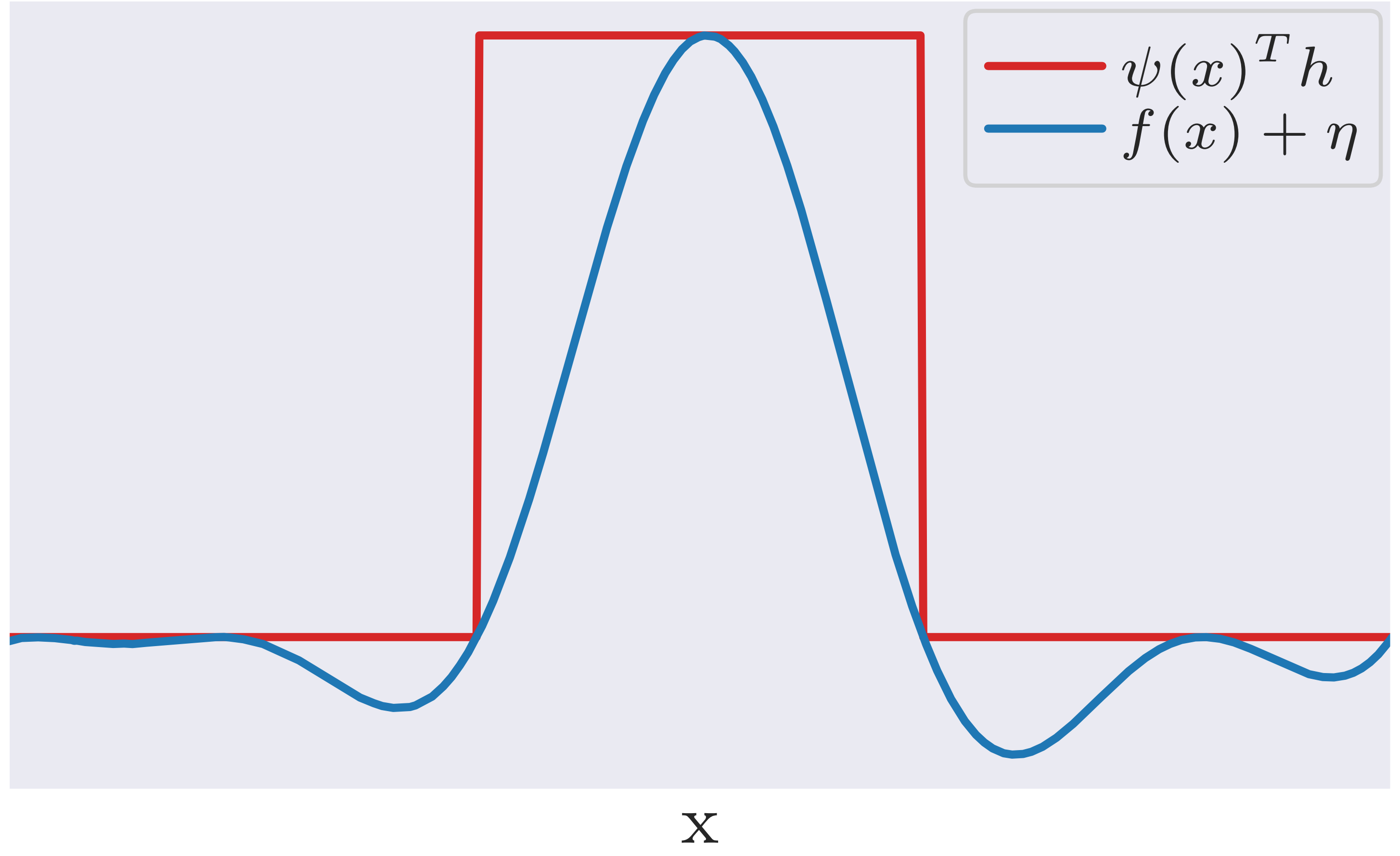
$$\text{s.t.} \quad f_0 + f(x,z) \le \psi(x;\theta)^T h(z) \quad \forall (x,z) \in \mathscr{X} \times \mathscr{Z} \,.$$

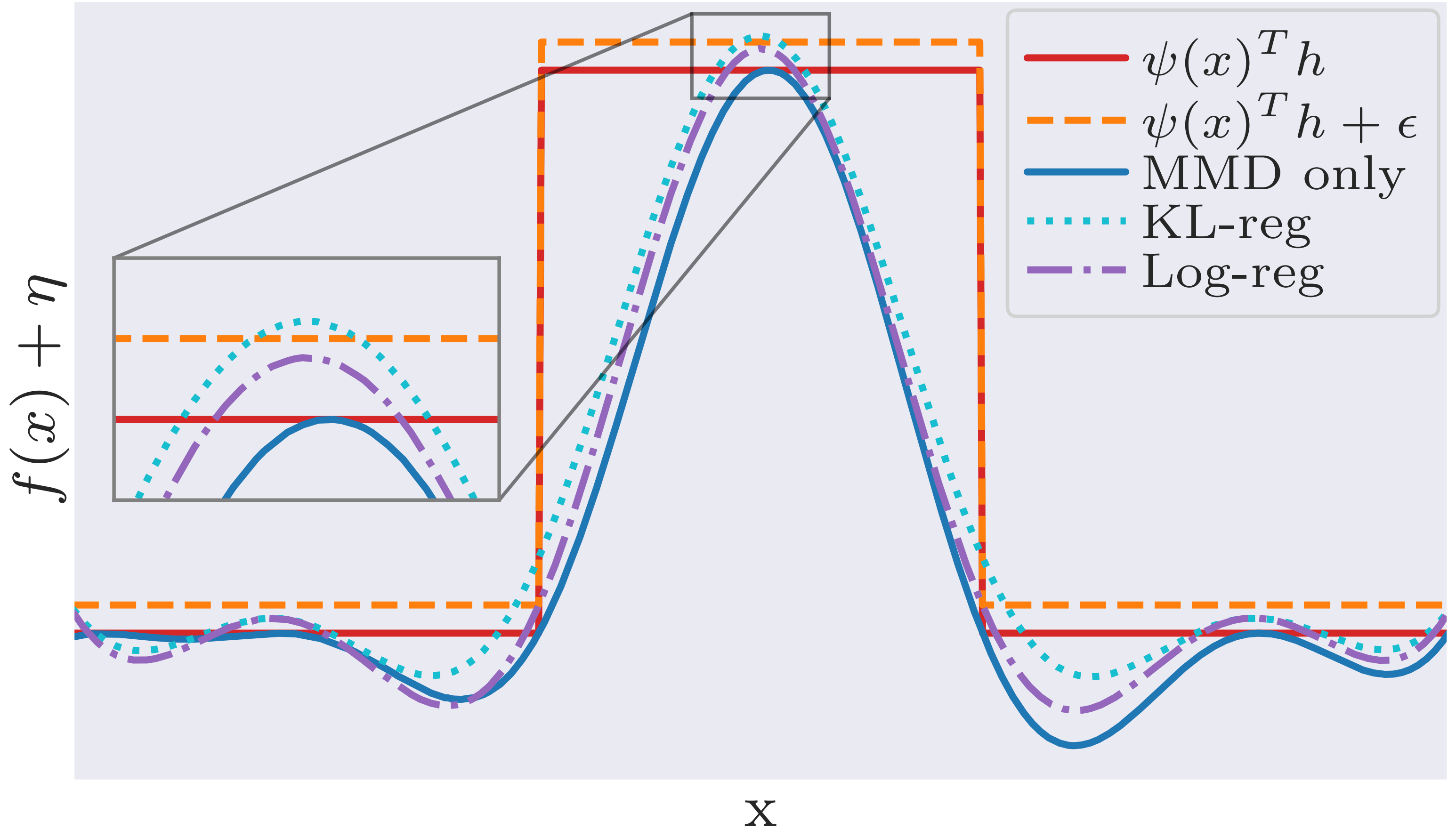
Entropy regularization Infinite constraint → soft-constraint

$$\inf_{\theta, Q \in \mathscr{P}} \frac{1}{2} \text{MMD}^2(Q, \hat{P}) + \lambda D_\phi(Q \| \omega) \;\; \text{s.t.} \;\; \mathbb{E}_Q \left[\psi(X;\theta)^T h(Z) \right] = 0$$

results in an unconstrained dual

$$\mathbb{E}_{\hat{P}_n}[f_0 + f(X,Z)] - \frac{1}{2}\|f\|_{\mathscr{F}}^2 - \mathbb{E}_\omega \left[\varphi_\epsilon^* \left(f_0 + f(X,Z) - \psi(X;\theta)^T h(Z) \right) \right]$$





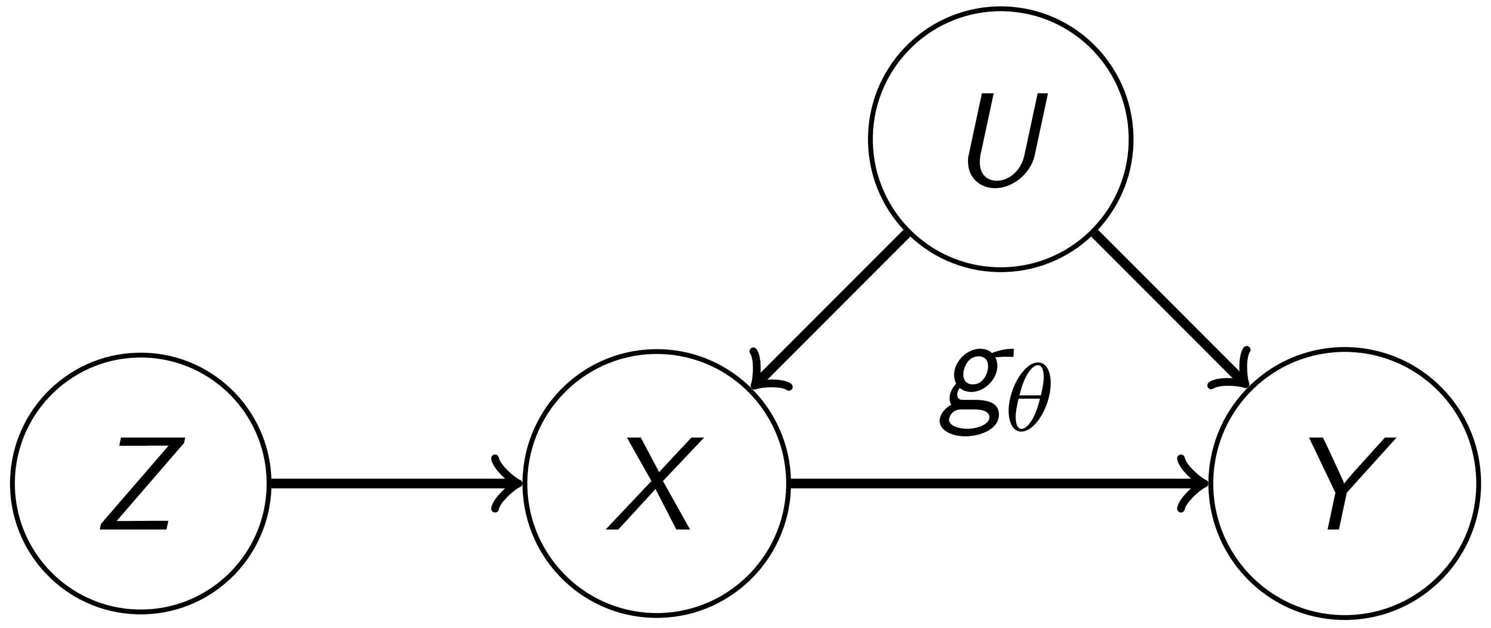
soft cons. $\phi_{\text{KL}}^*(t) = \exp(t)$

log-barrier $\phi_{\log}^*(t) = -\log(1-t)$

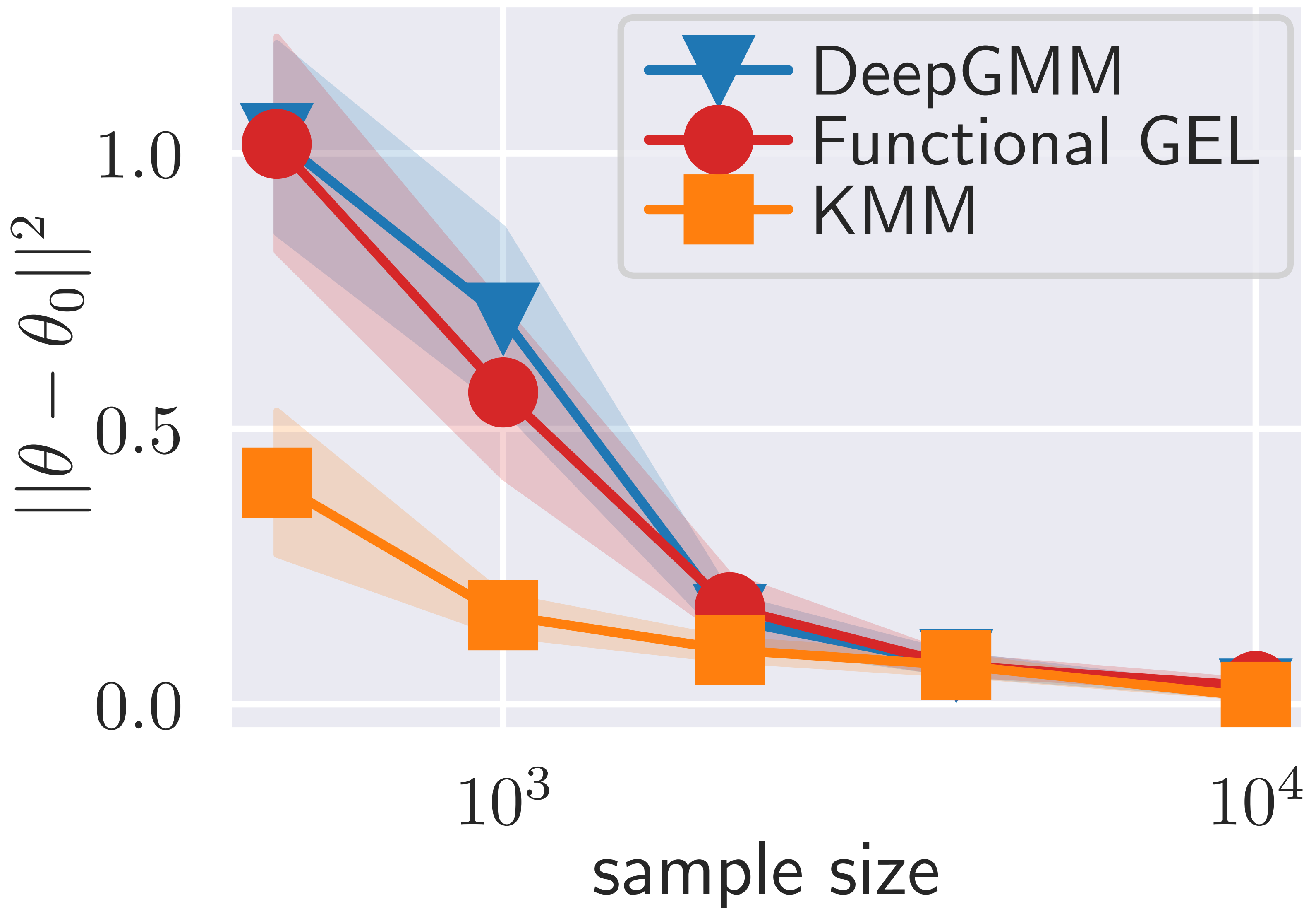
Kernel MoM: Nonlinear Instrumental Variable Regression

$$Y := g(X;\theta_0) + \nu(U) + \epsilon_1$$
$$X := \eta(Z) + \mu(U) + \epsilon_2 \qquad ,$$
$$Z \sim P_Z, \quad \epsilon_{1/2} \sim \mathcal{N}(0,\sigma)$$

$g(x;\theta)$ is nonlinear in both x, θ.



Estimate θ using Kernel MoM with CMR

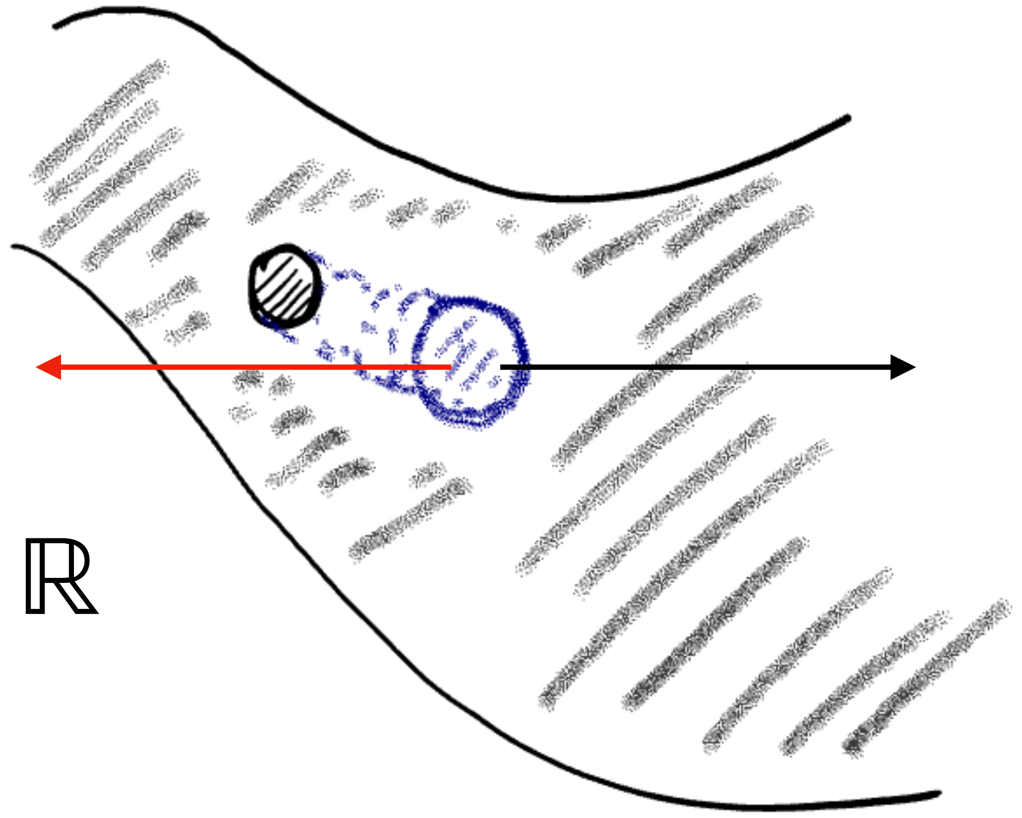


Takeaway. (Strong) structured distribution shifts (e.g., causal confounding) can be accounted for using the Kernel MoM + CMR, but not (joint) DRO, adversarial robustness, …

Force-balance of Kernel MoM

Lagrangian: $$\sup_{\gamma\in\mathbb{R},h\in\mathscr{H}} \boxed{\inf_{Q} \frac{1}{2}\mathrm{MMD}^2(Q,\hat{P}) + \gamma\cdot\mathbb{E}_Q\left[\left(Y-g_\theta(X)\right)^T h(Z)\right]}$$

Minimizing movement scheme (MMS) in MMD $\inf_{\mu\in\mathscr{P}} F(\mu)+\frac{1}{2\gamma}\mathrm{MMD}^2(\mu,\mu^k)$



Force balance using **function approximation**, e.g., kernel functions

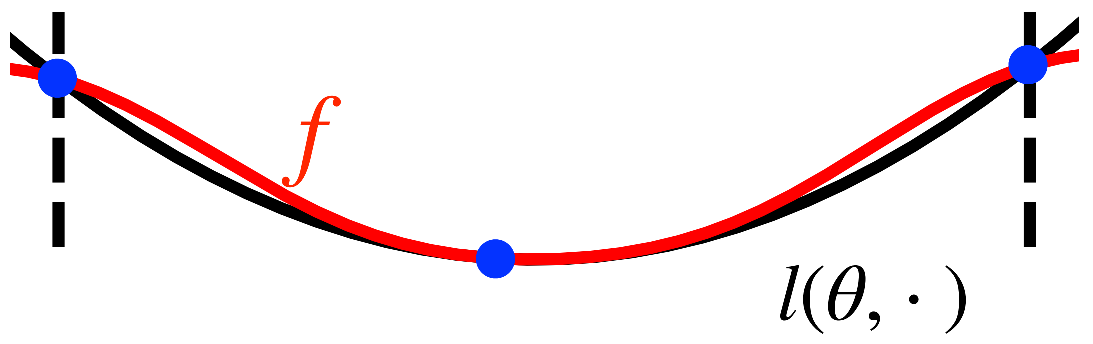
$$-\mathrm{D}F = f+f_0,\quad f=\frac{1}{\tau}\sum_{i=1}^{n}\alpha_i k([x_i,y_i,z_i],\cdot\,)\in\mathscr{H}, f_0\in\mathbb{R}$$

Since $\mathrm{D}F = \left(Y-g_\theta(X)\right)^T h(Z)$, the optimal force function approximates the moment function

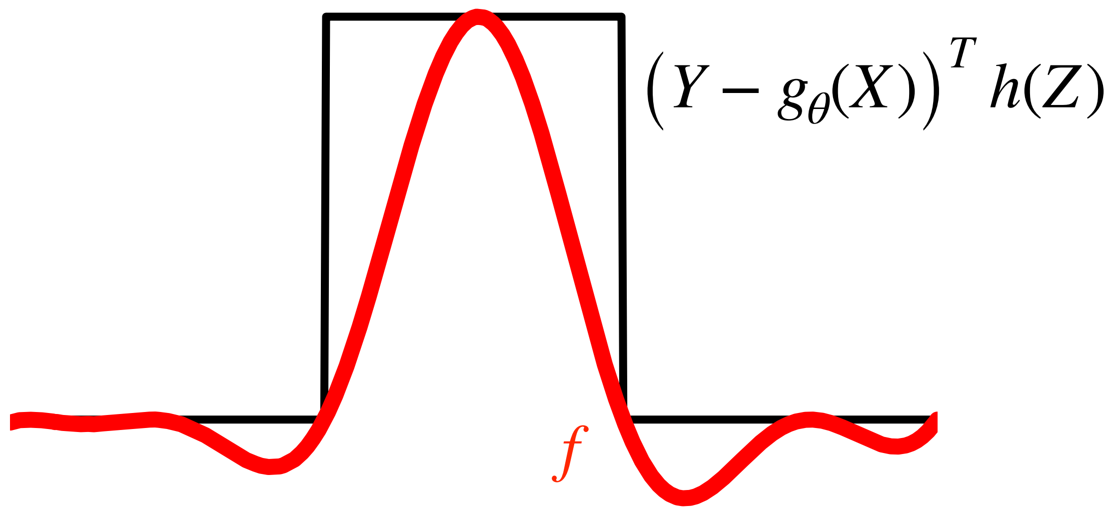
$$f+f_0=\left(Y-g_\theta(X)\right)^T h(Z)\ \text{a.e.}$$

Summary

- We exploited explicitly parametrized **dual force functions** for **robust learning** under **joint** and **structured distribution shifts**. This is inspired by **generalized force** in gradient flows, optimal transport, and mechanics.
- The gradient flow force-balance eqns give insights for constructing robust learning algorithms.
  - **Kernel DRO**: force gives the robustified surrogate loss



  - **Kernel MoM**: force gives the robustified moment function



This talk is mainly based on:

1. **Z.**, Jitkrittum, W., Diehl, M. & Schölkopf, B. Kernel Distributionally Robust Optimization. AISTATS 2021
2. Kremer, H., Nemmour, Y. , Schölkopf, B. & **Z**. Estimation Beyond Data Reweighting: Kernel Method of Moments. ICML 2023

slides & code available: jj-zhu.github.io

Postdoc position opening in Berlin: data-driven dynamics modeling for medical imaging. Contact for info.