

Duality from Distributionally Robust Learning to Gradient Flow Force-Balance

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Weierstraß-Institut für
Angewandte Analysis und Stochastik

Duality in this talk: Measures vs Functions

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Primal-dual optimization problems

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Examples

Generative models

$$\inf_{G_\theta} \mathbb{E}_Z \mathcal{D}(P, G_\theta(Z)) = \inf_{\mu \in \mathcal{M}} \sup_{f \in \mathcal{F}} \left\{ \int f(x) dP(x) - \mathbb{E}_{\theta \sim \mu} \int f(g_\theta(z)) dQ(z) \right\}$$

Distributionally robust optimization

$$\inf_{\theta} \sup_{\substack{\mu \\ \text{MMD}(\mu, \hat{\mu}) \leq \epsilon}} \mathbb{E}_{\mu}[l(\theta; x)] = \inf_{\theta \in \mathbb{R}^d, f \in \mathcal{H}} \sup_{\mu \in \mathcal{M}} \mathbb{E}_{\mu}(l - f) + \frac{1}{N} \sum_{i=1}^N f(x_i) + \epsilon \|f\|_{\mathcal{H}}.$$

Wasserstein barycenter

$$\min_{\mu \in \mathcal{M}} \sum_{i=1}^n \alpha_i [W_p(\mu, \nu_i)] = \min_{\mu \in \mathcal{M}} \sum_{i=1}^n \alpha_i \sup_{f_i \in \Psi_c} \left\{ \int f_i^c d\mu + \int f_i d\nu_i \right\},$$

Static: Duality of Distributionally Robust Learning

Distributional robustness, but what kind?

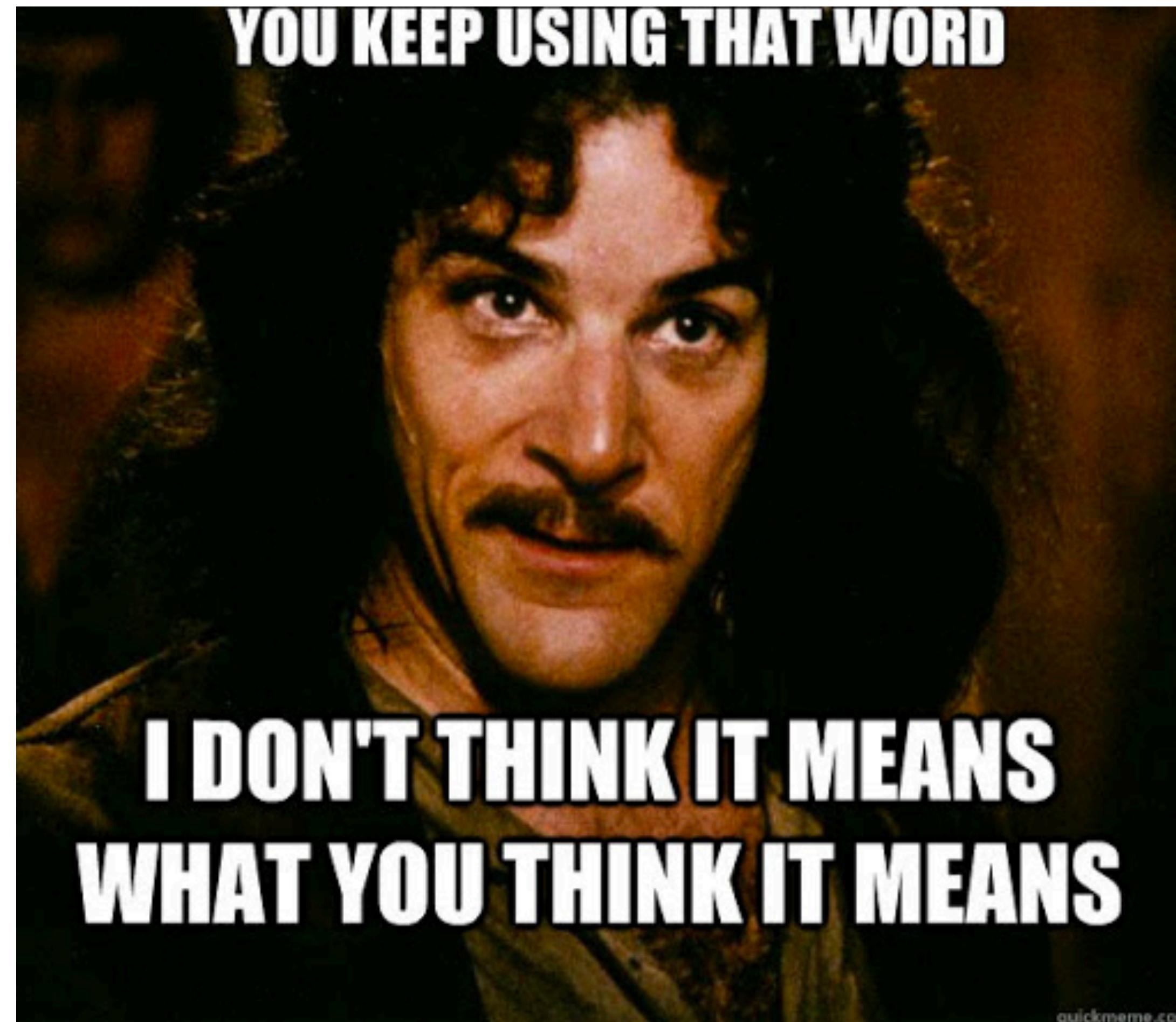


Figure credit: The Princess Bride,
a bedside story by your grandpa

From Statistical Learning to Distributionally Robust Learning

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Empirical Risk Minimization

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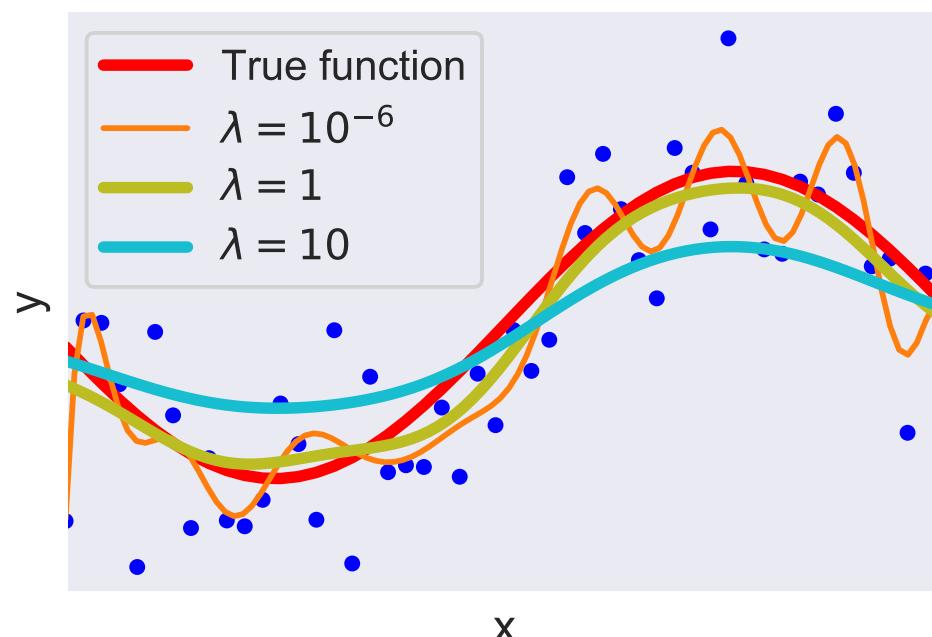
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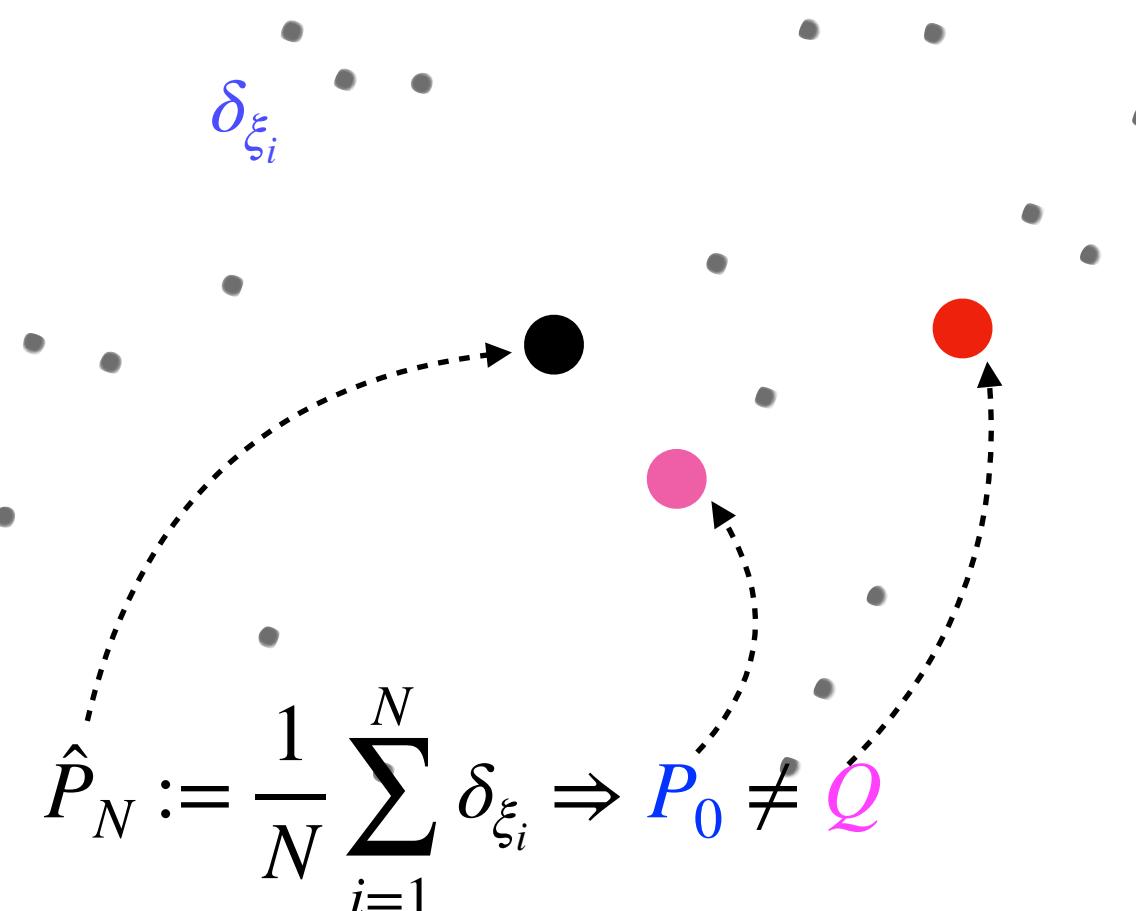
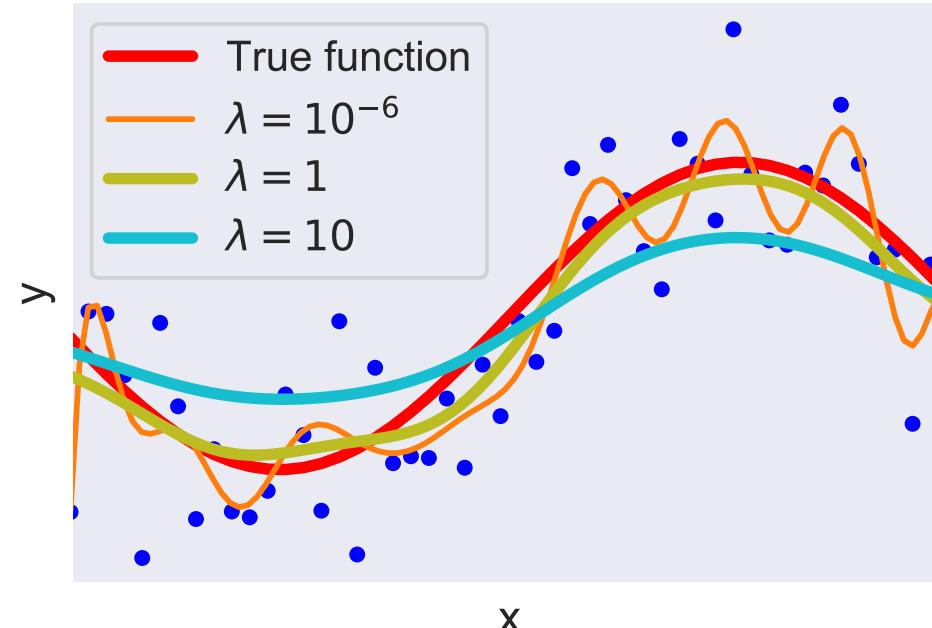
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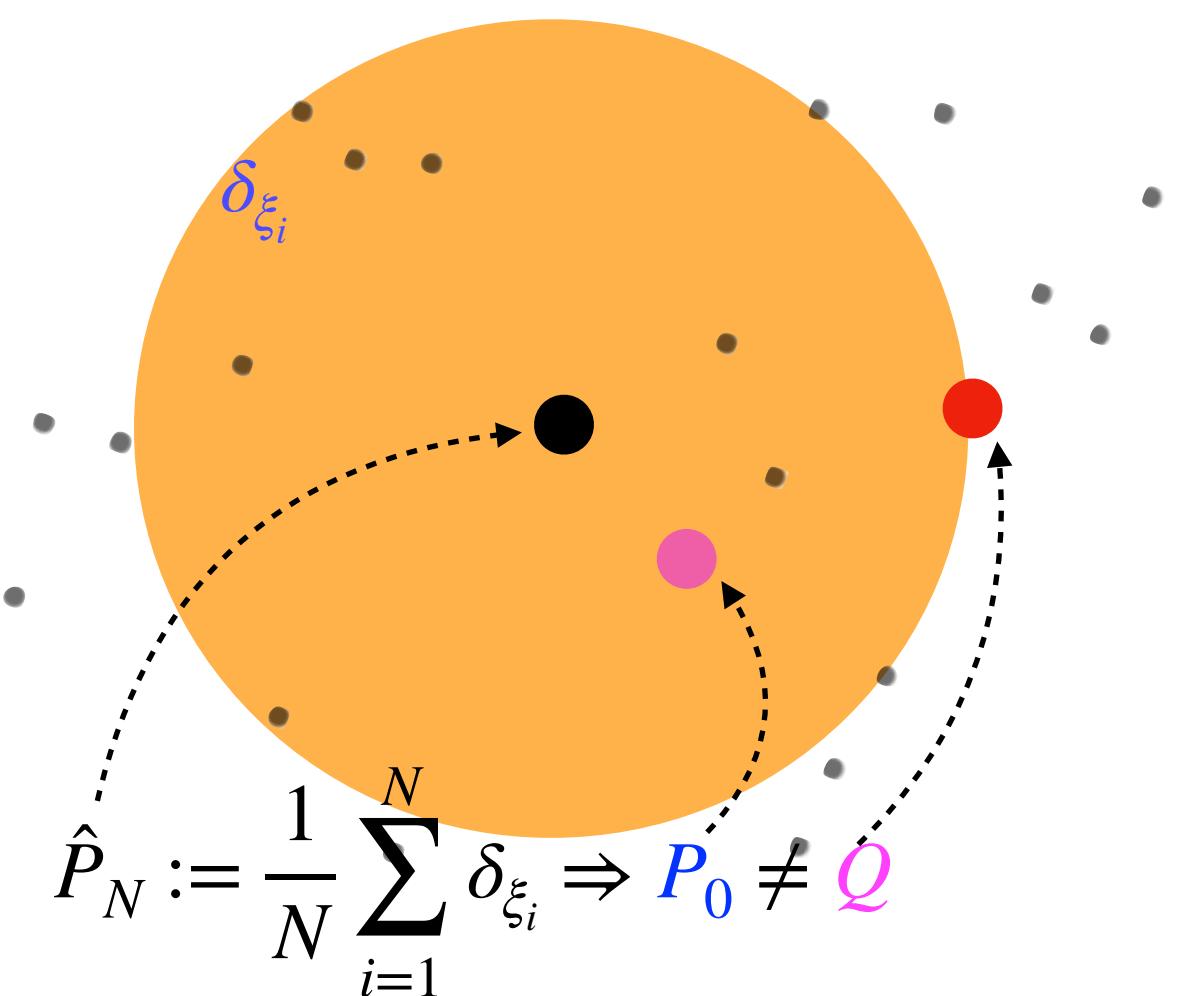
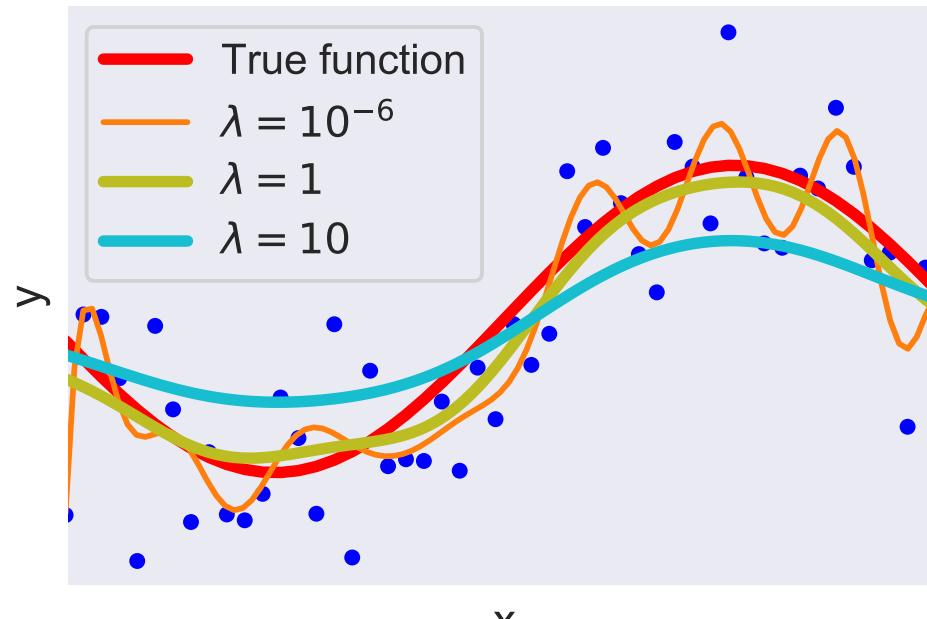
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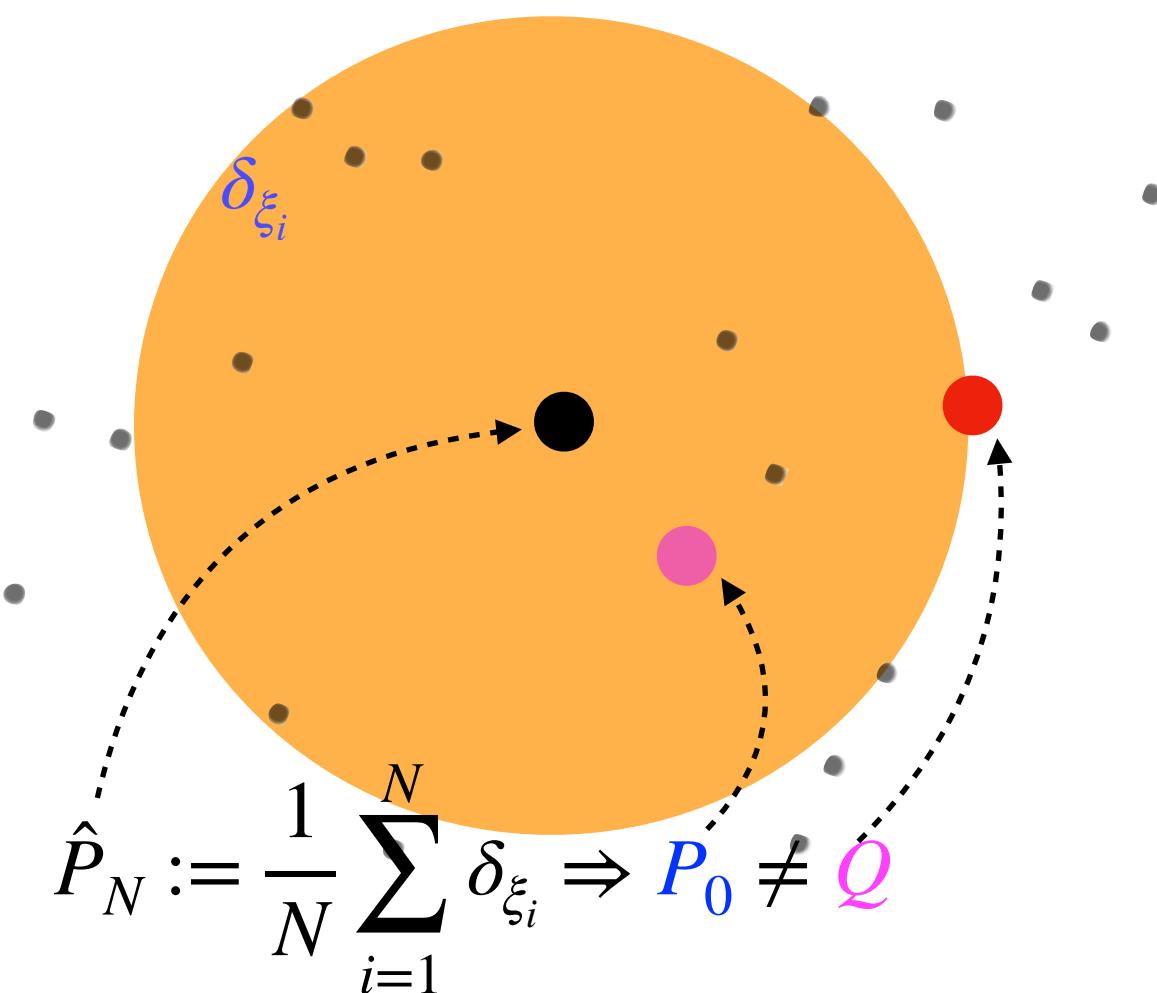
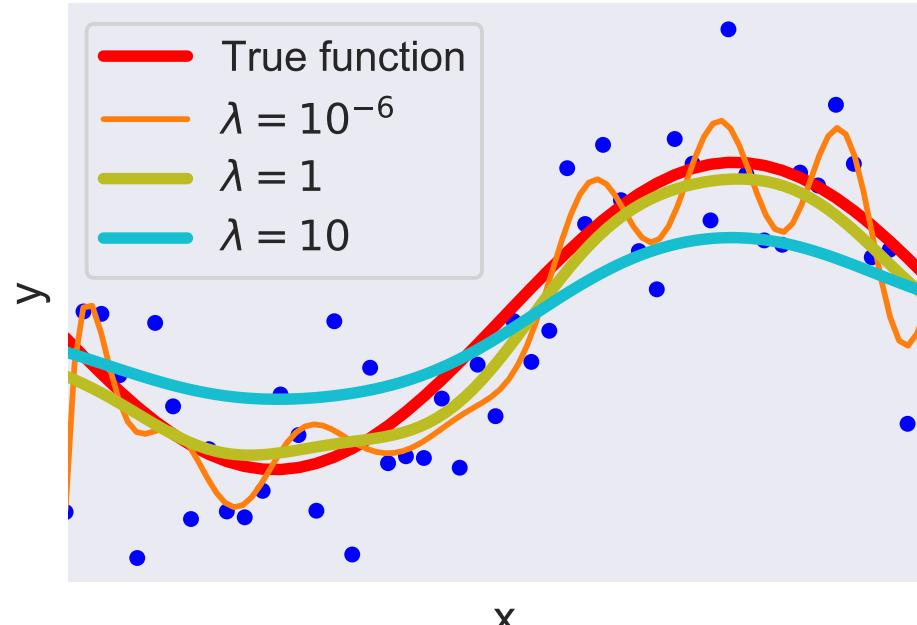
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[Delage & Ye 2010] in certain geometry.

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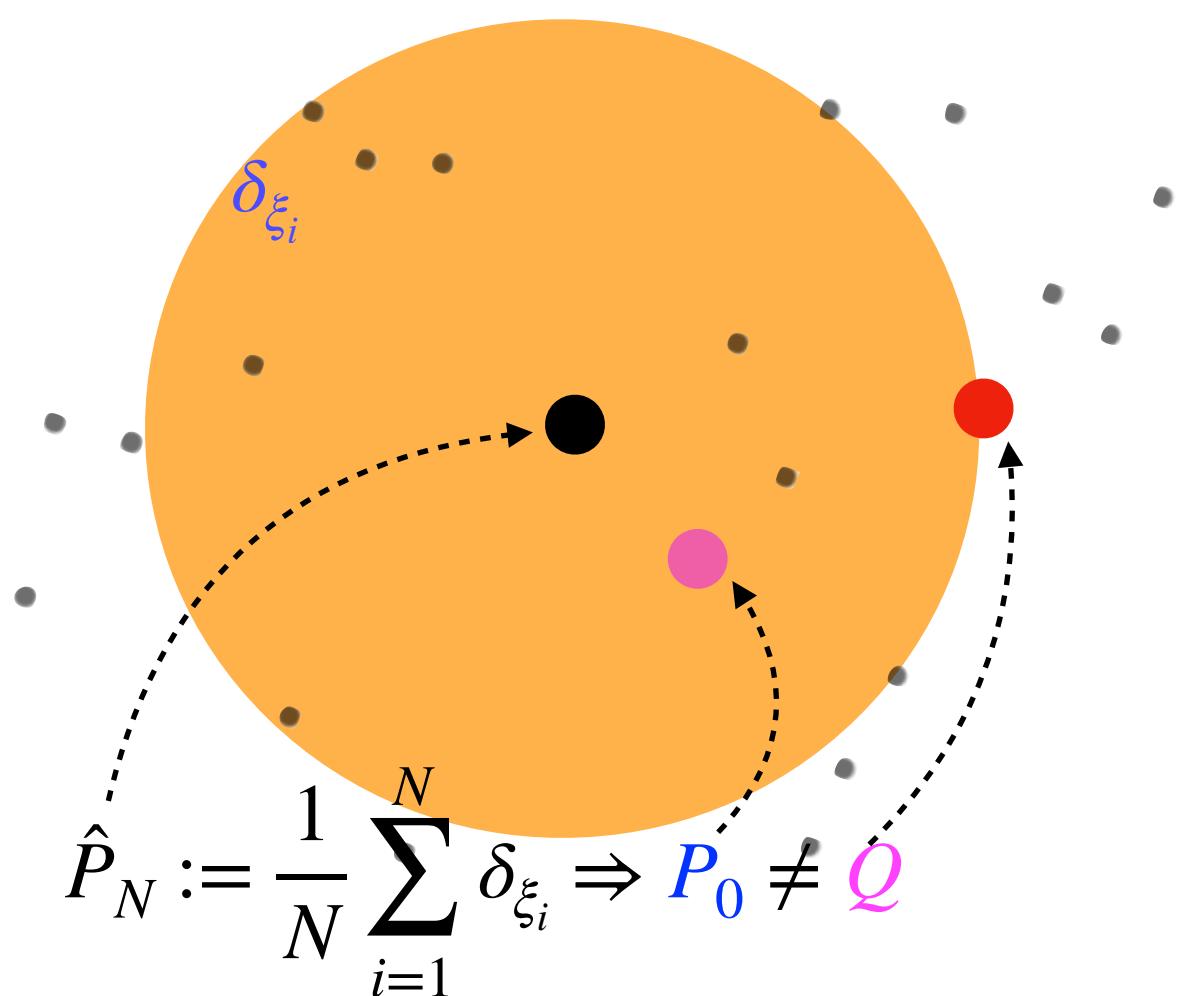
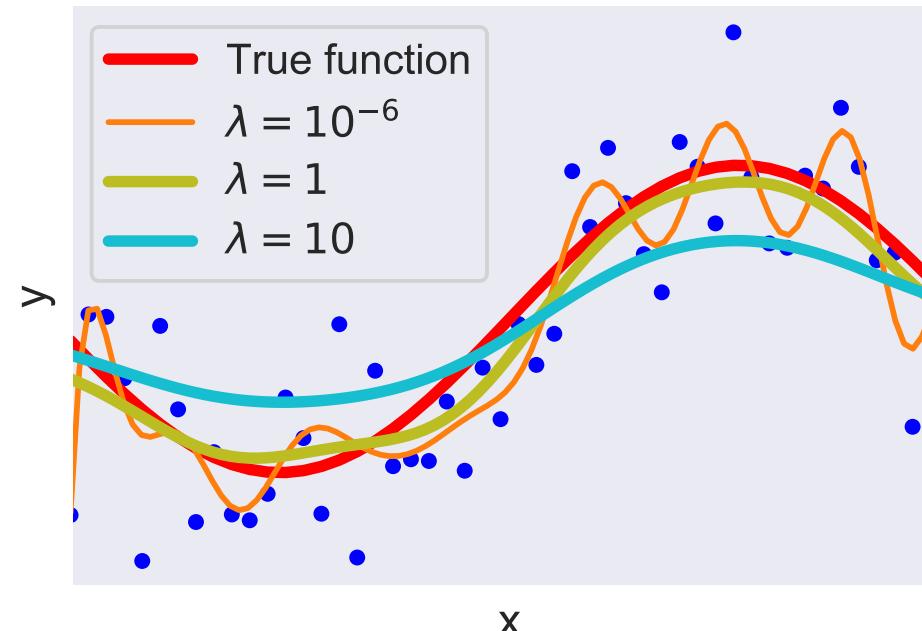
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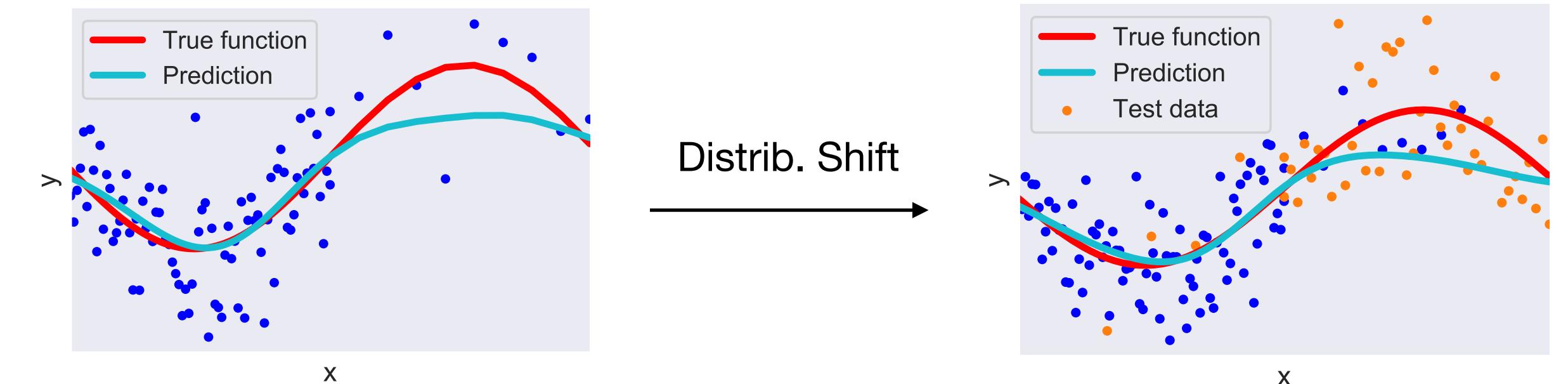
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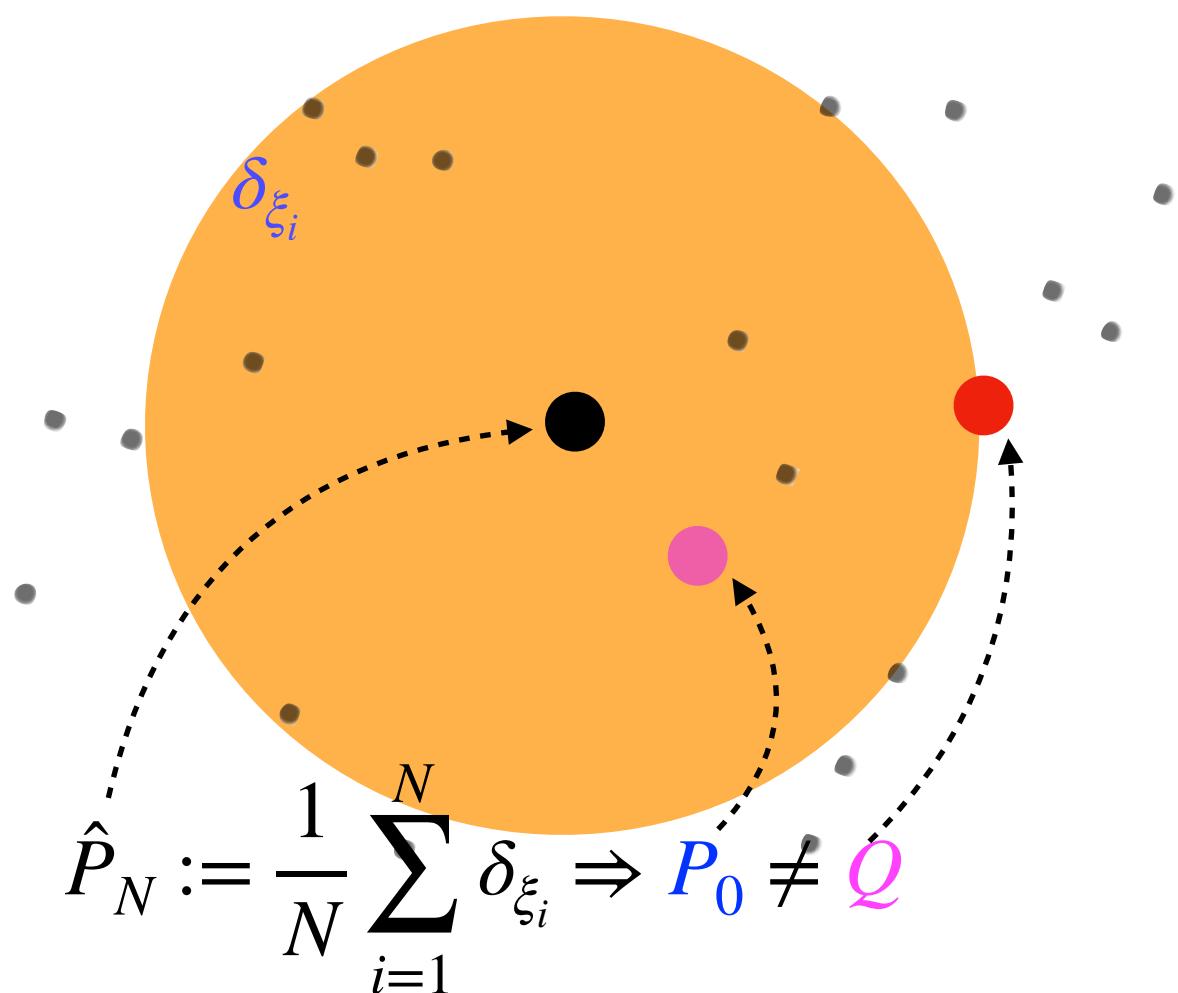
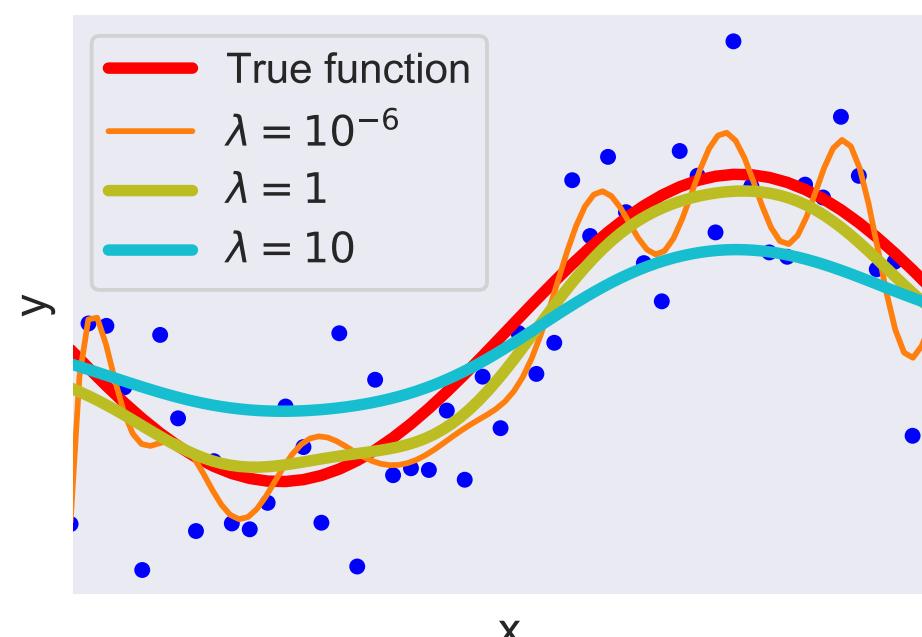
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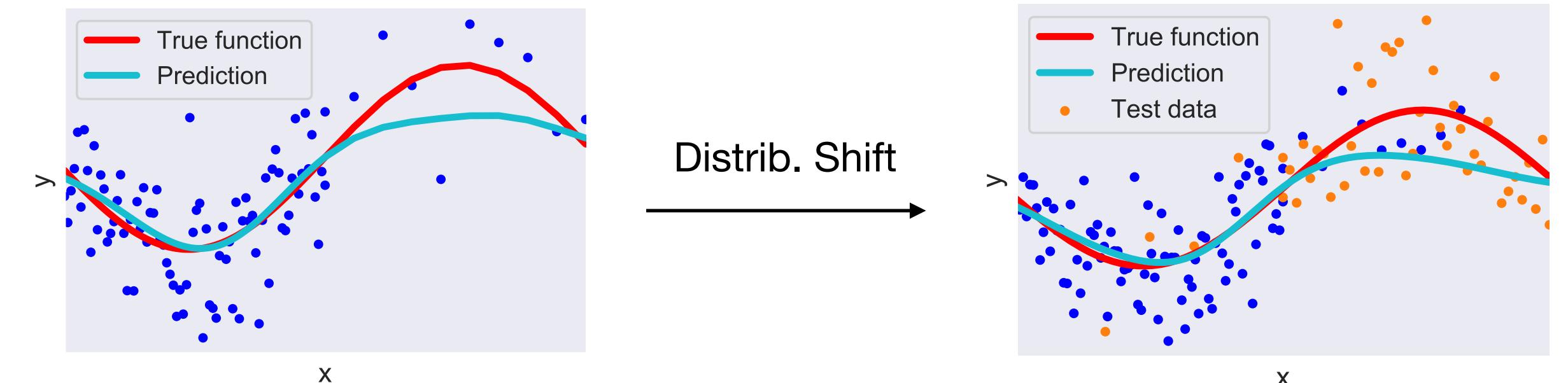
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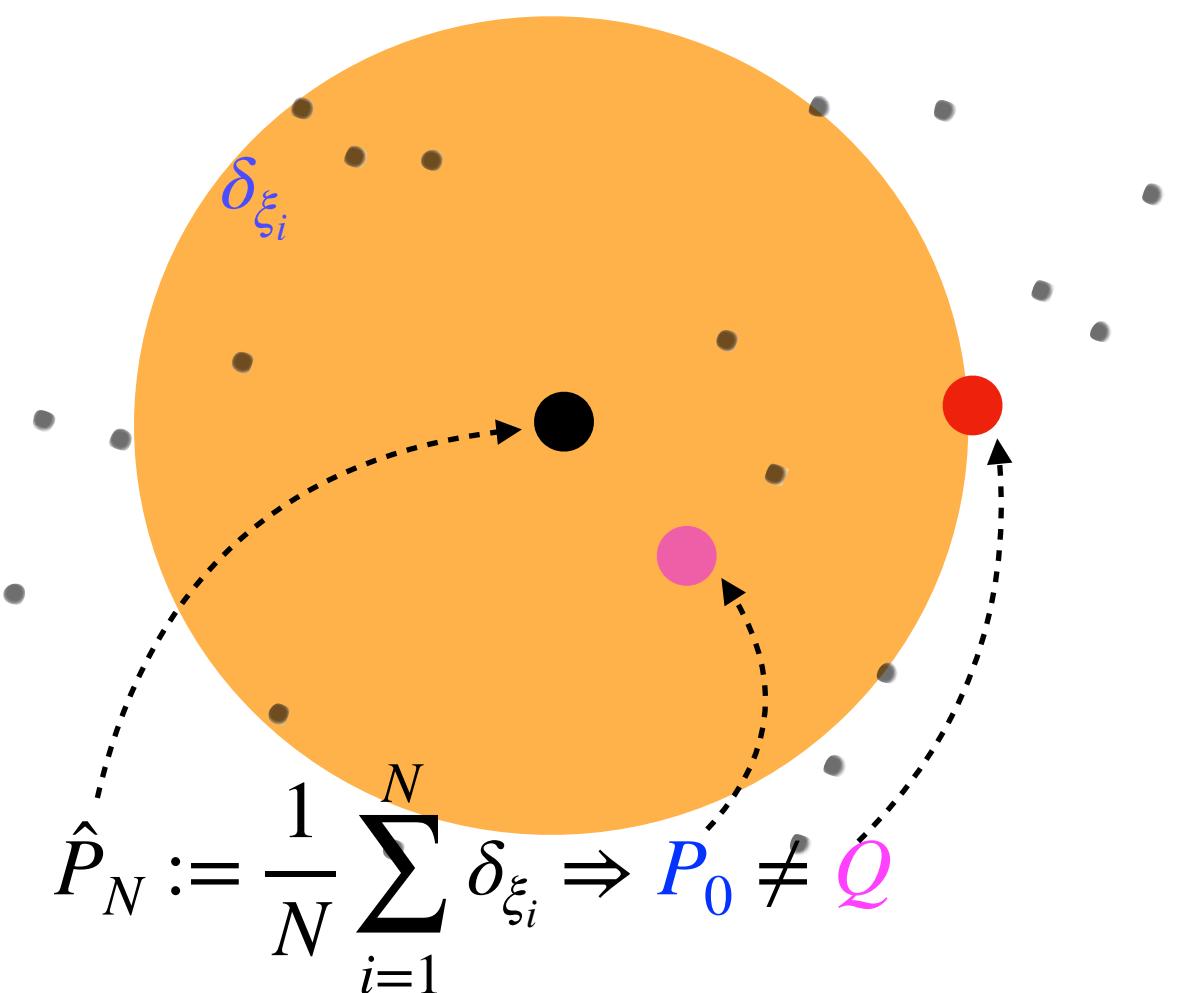
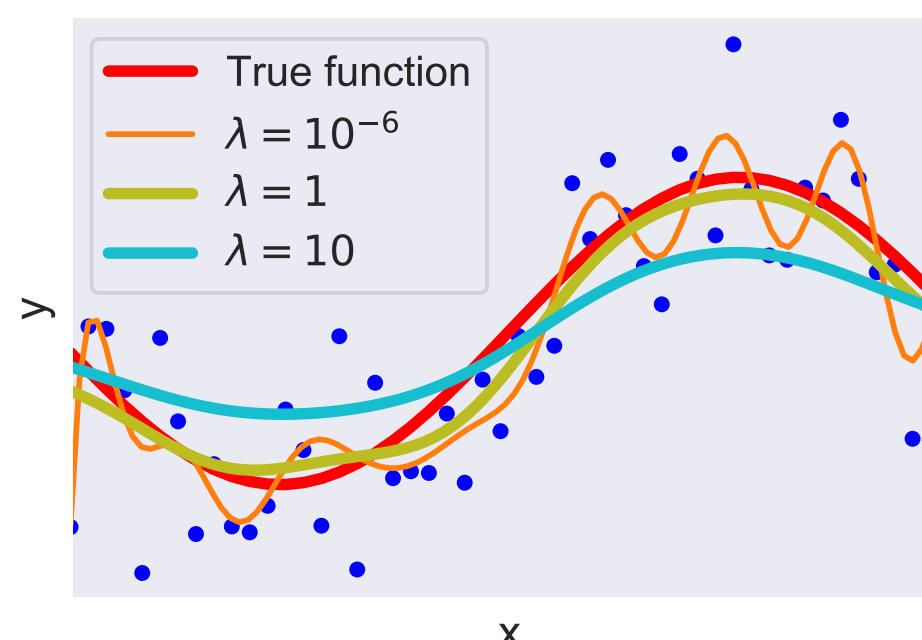
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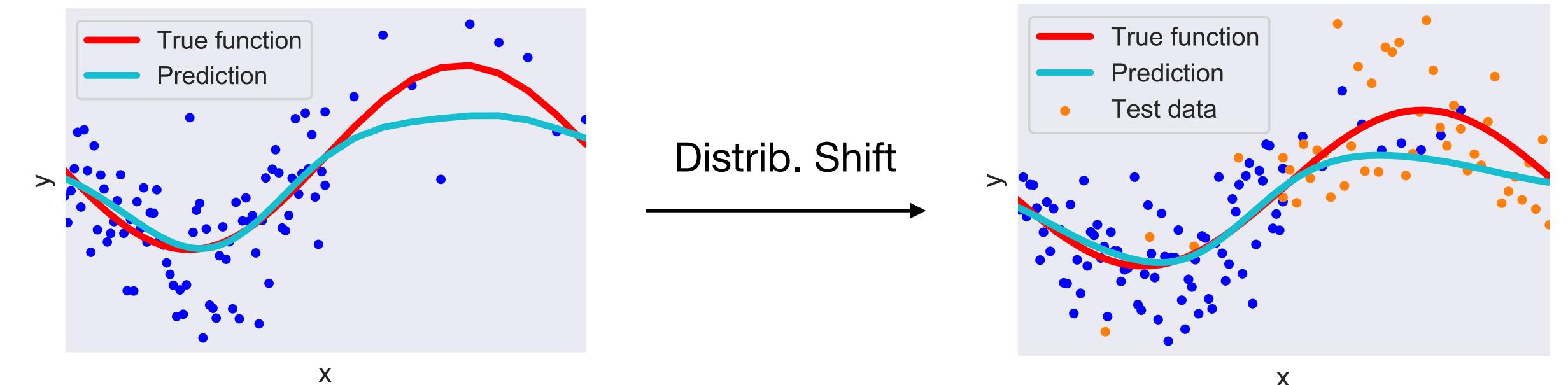
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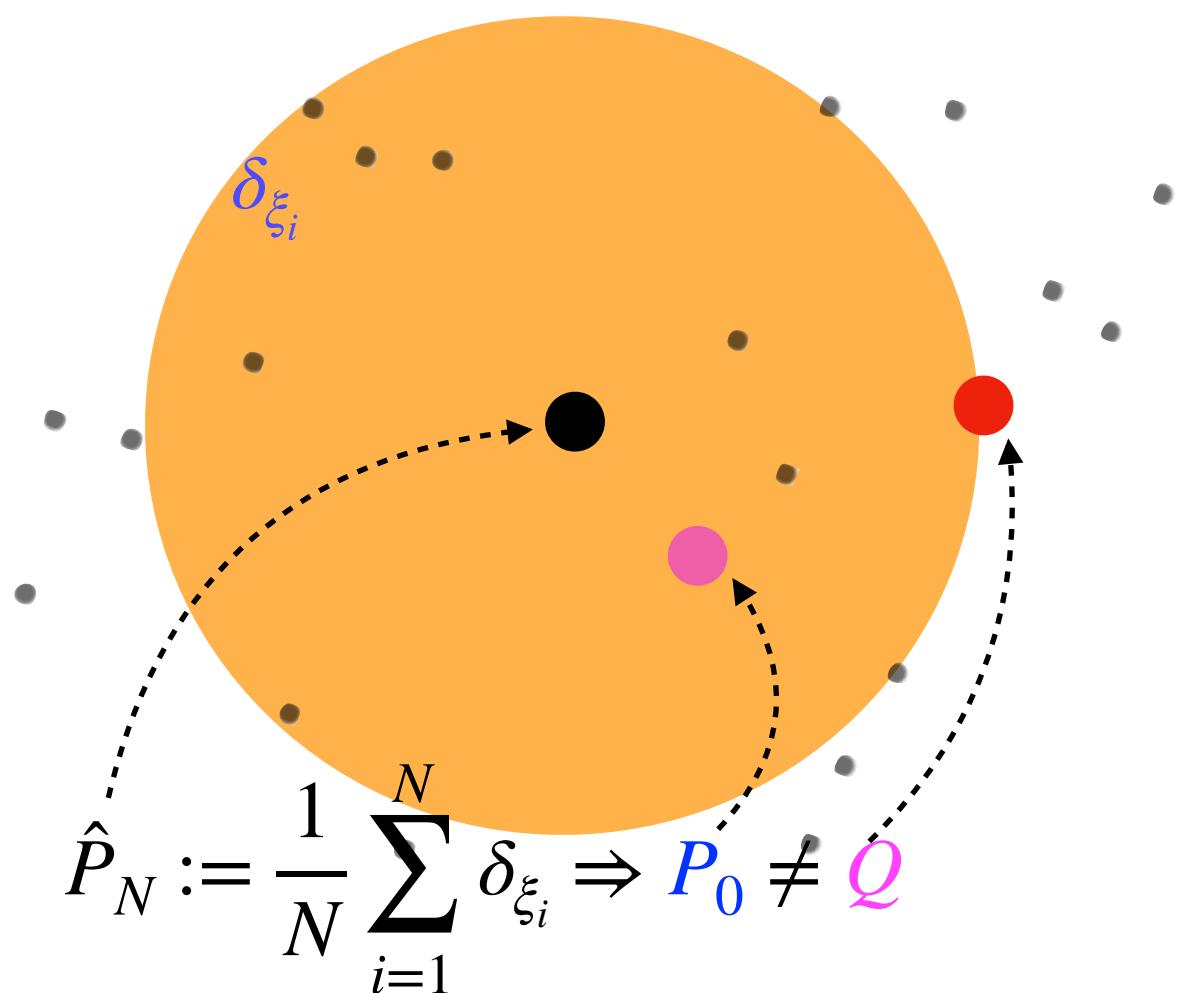
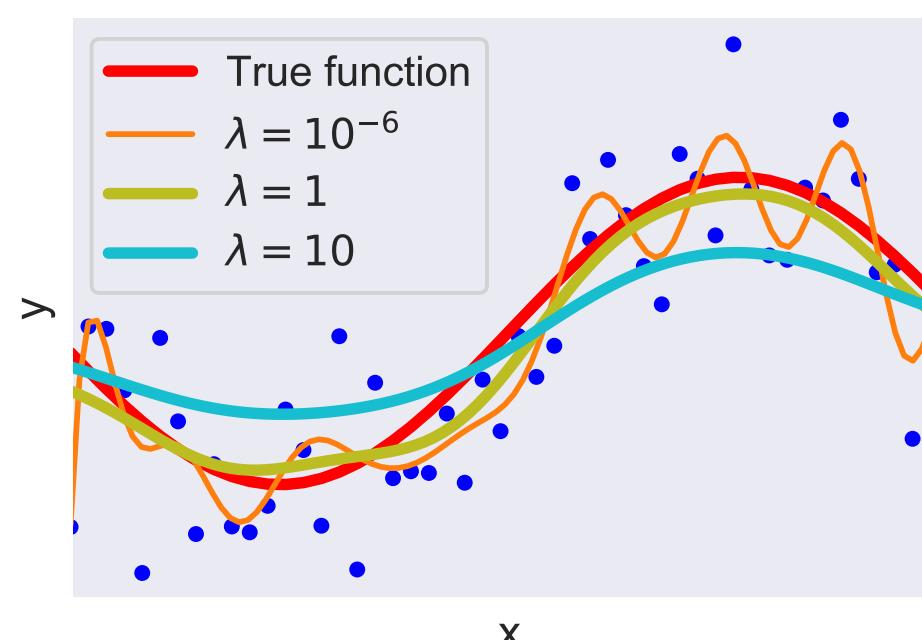
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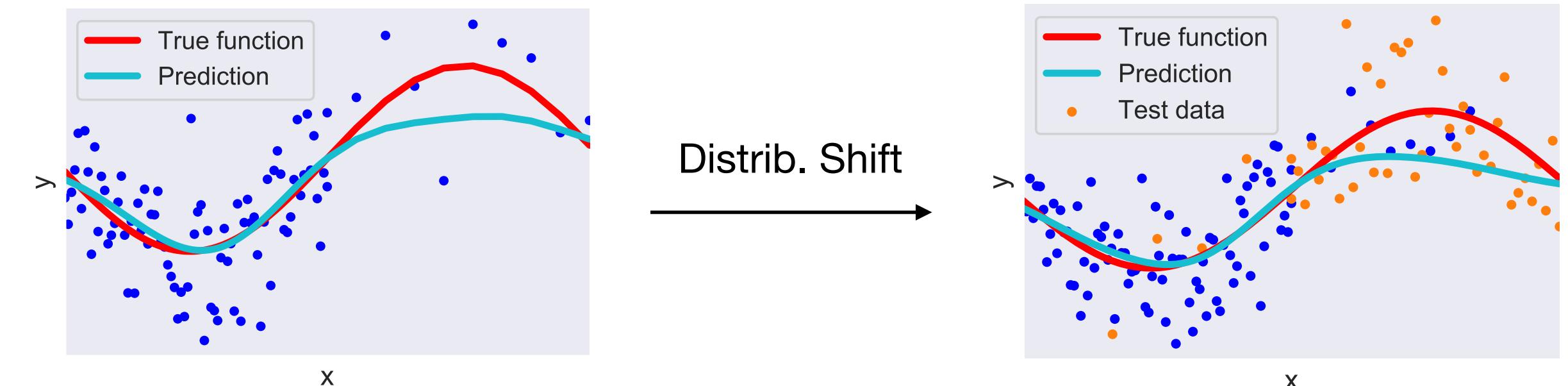
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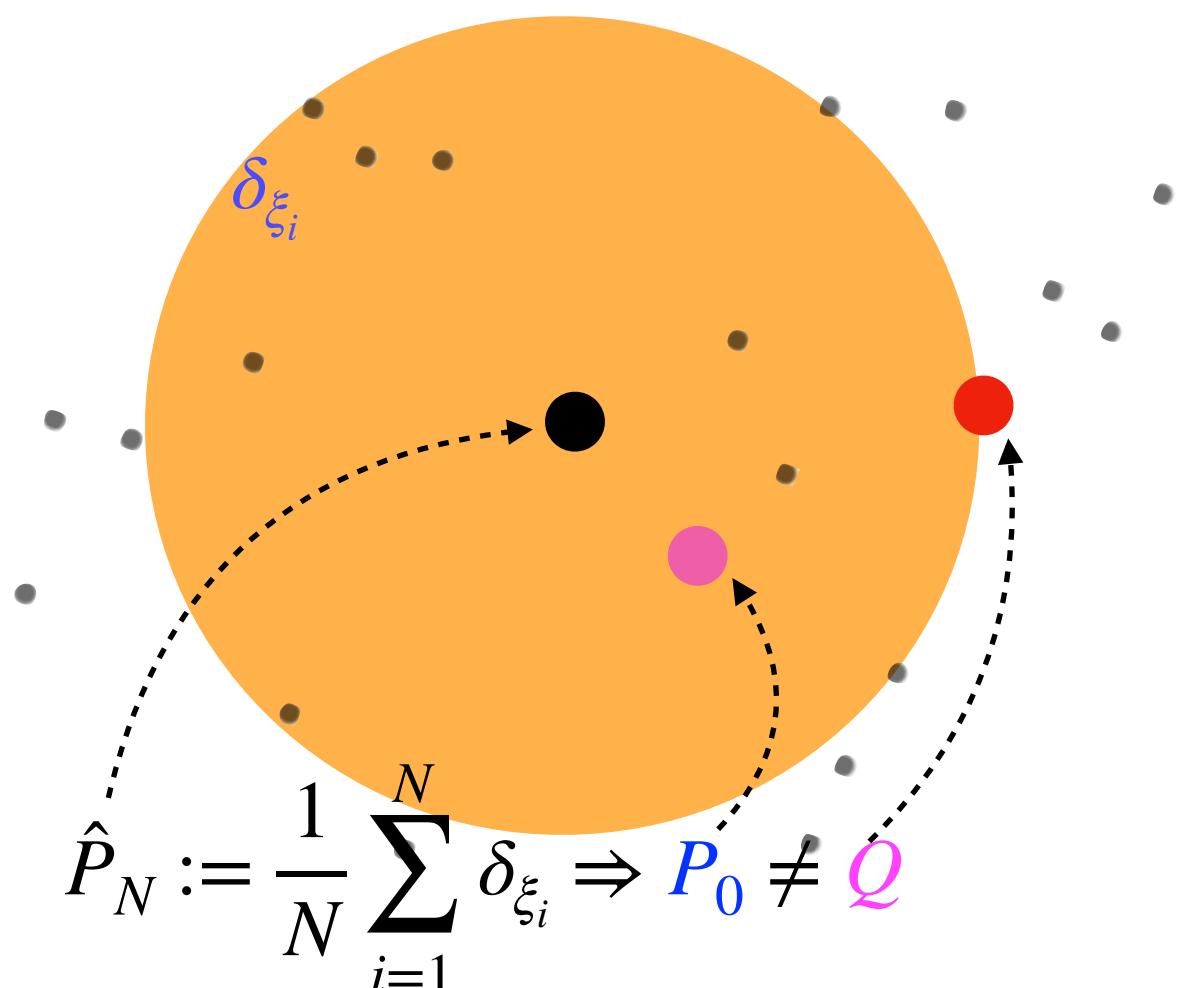
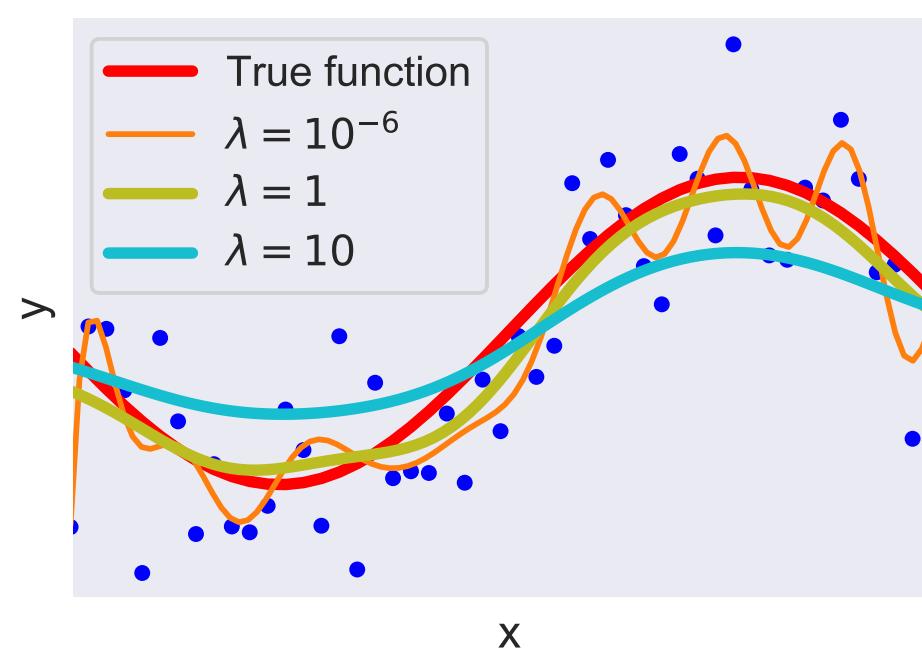
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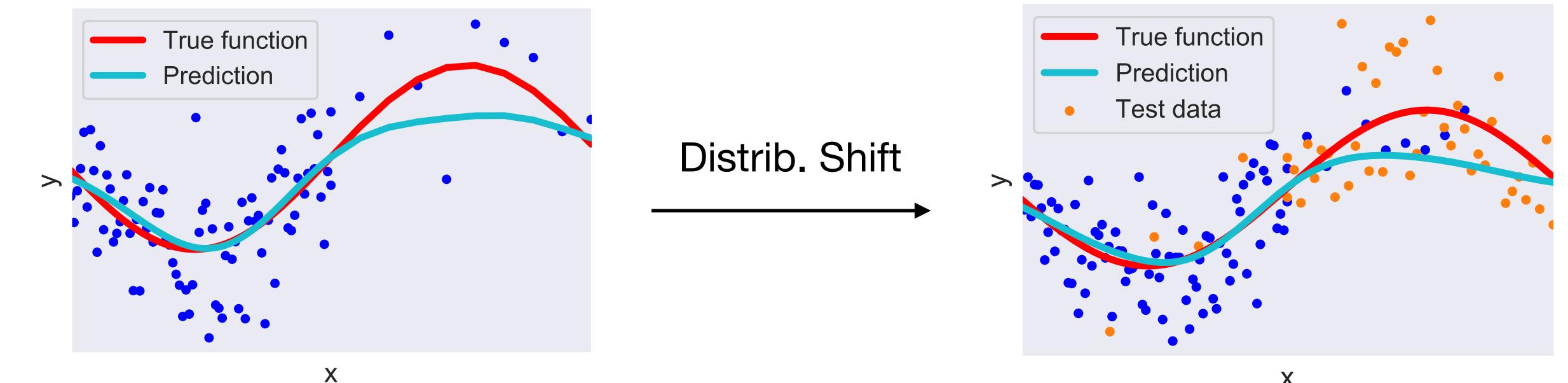
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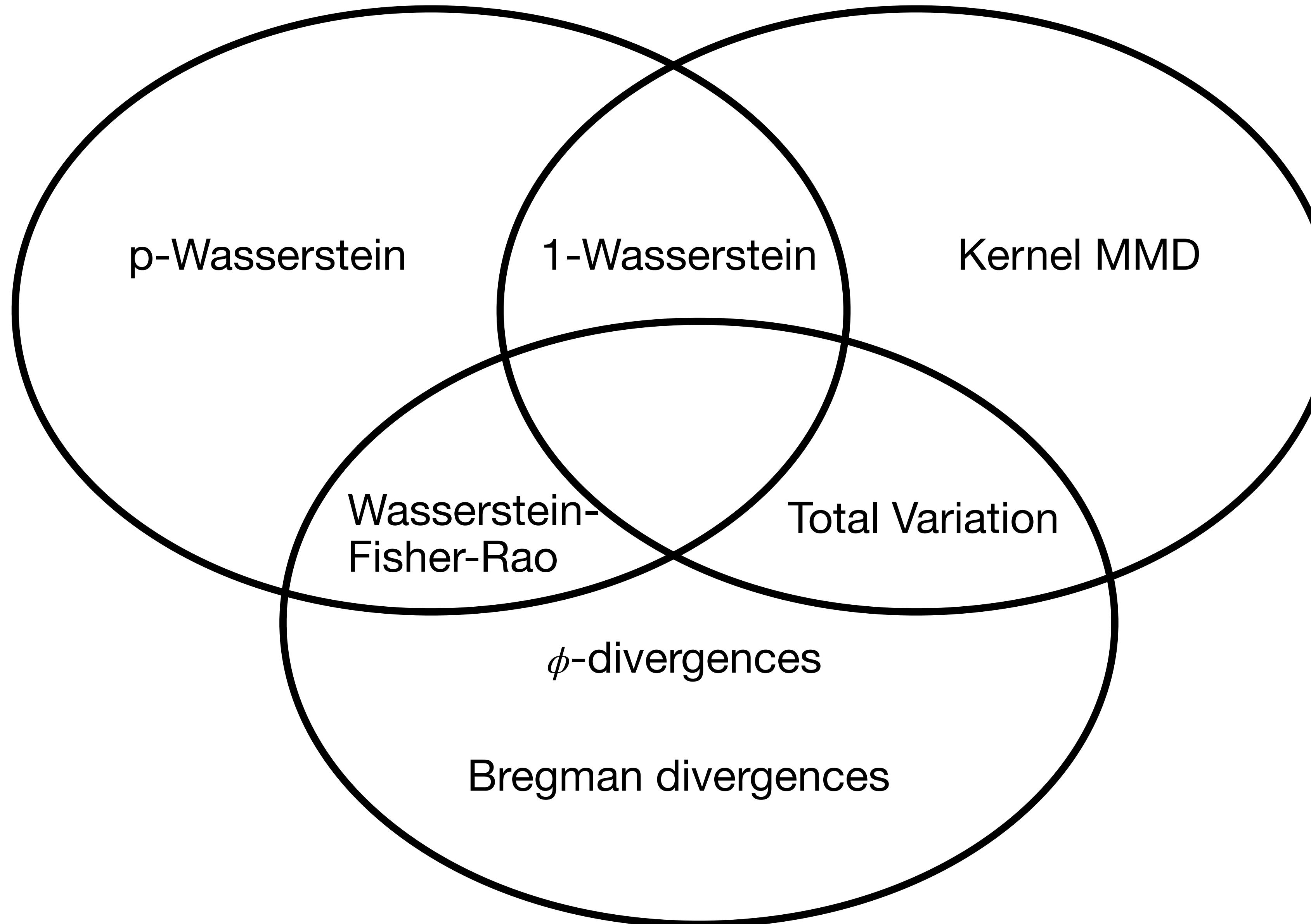
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Wasserstein Gradient flow [F. Otto et al.] e.g. Fokker-Planck equation as Wasserstein flow

Figure credit: H. Kremer

Optimal Transport

Integral Prob. Metrics

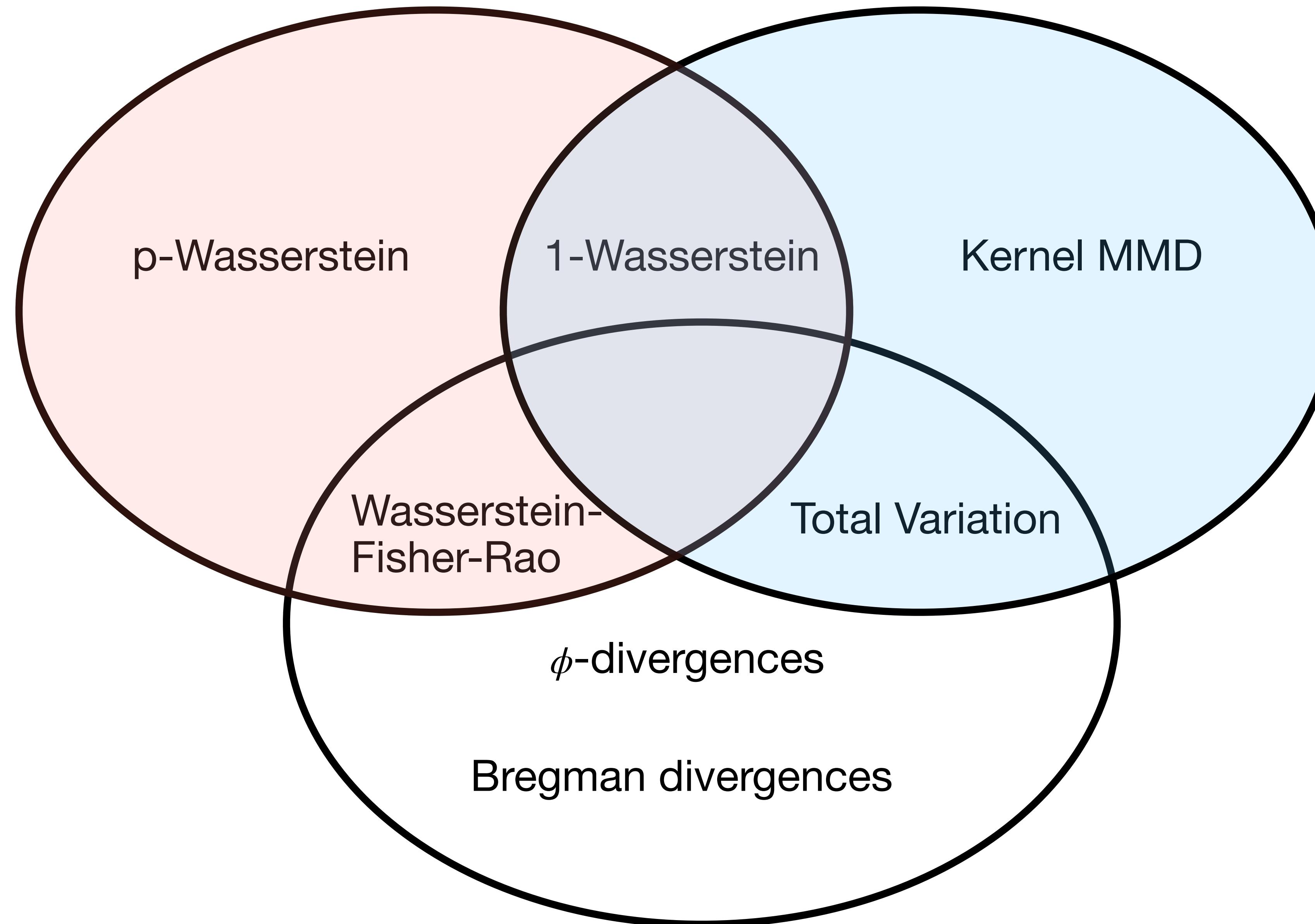


Information Divergence

Figure credit: J. Zhu

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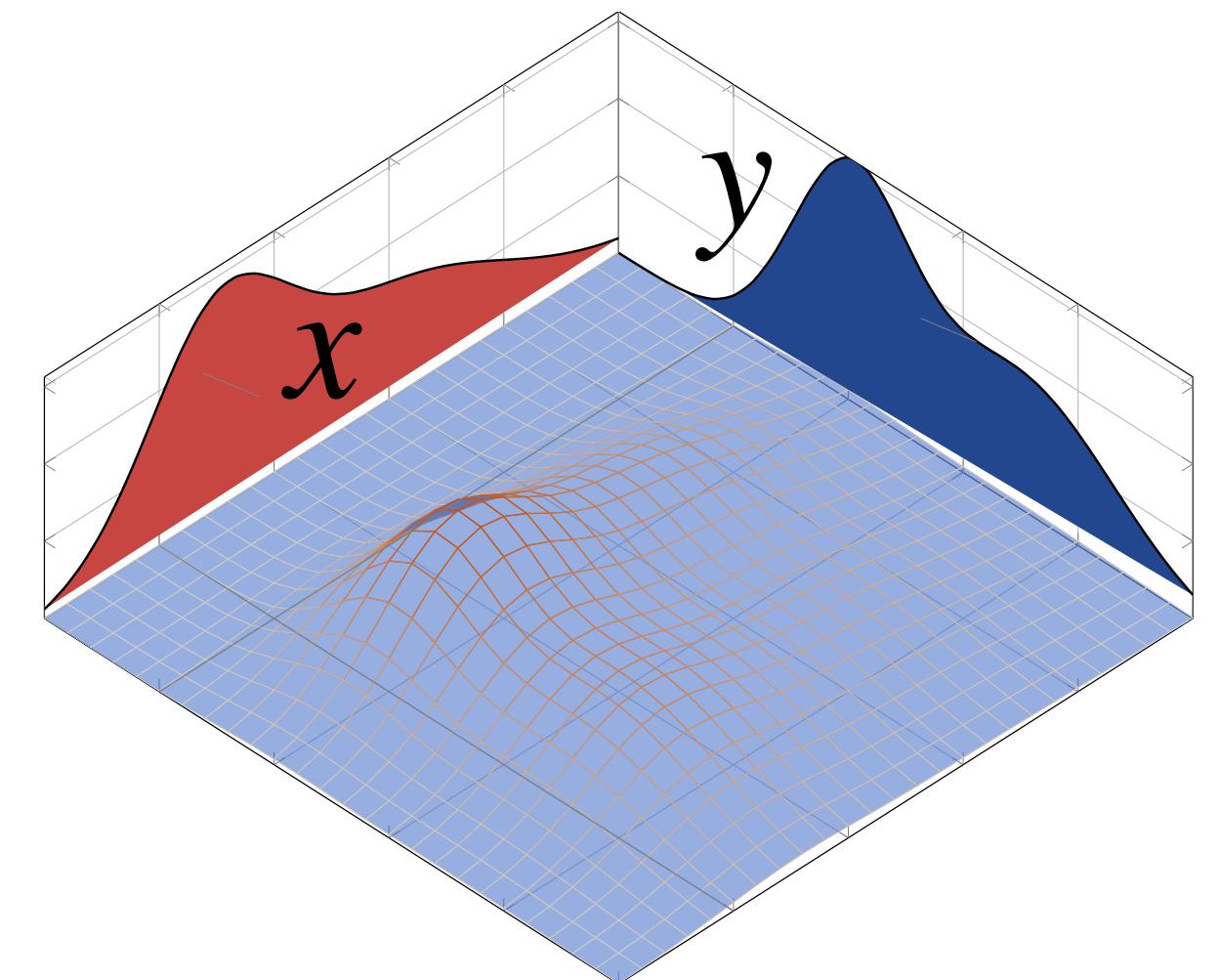
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Definition. The p -**Wasserstein distance** between probability measures P, Q on \mathbb{R}^d (with p finite moments, $p \geq 1$) is defined through the following Kantorovich problem

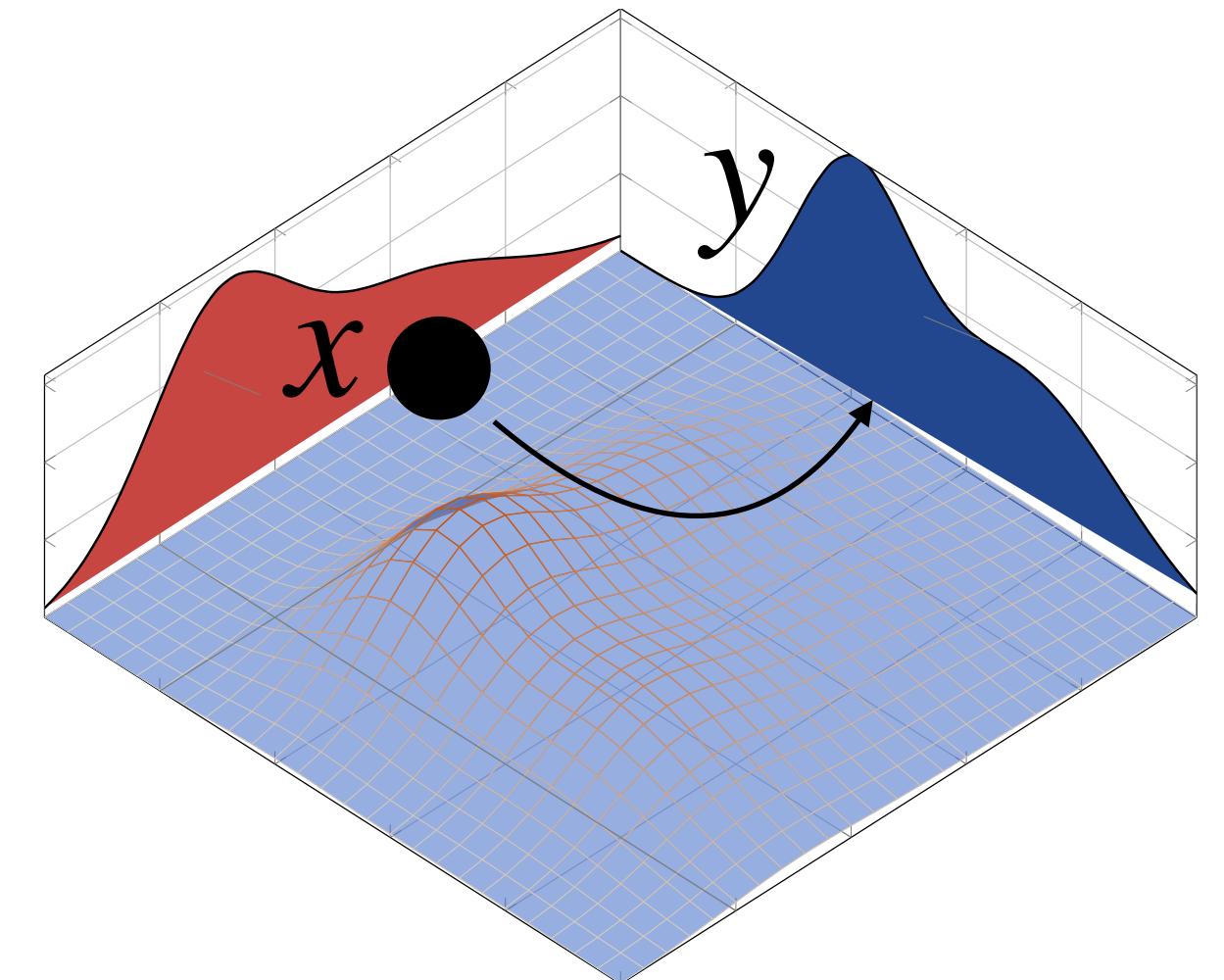
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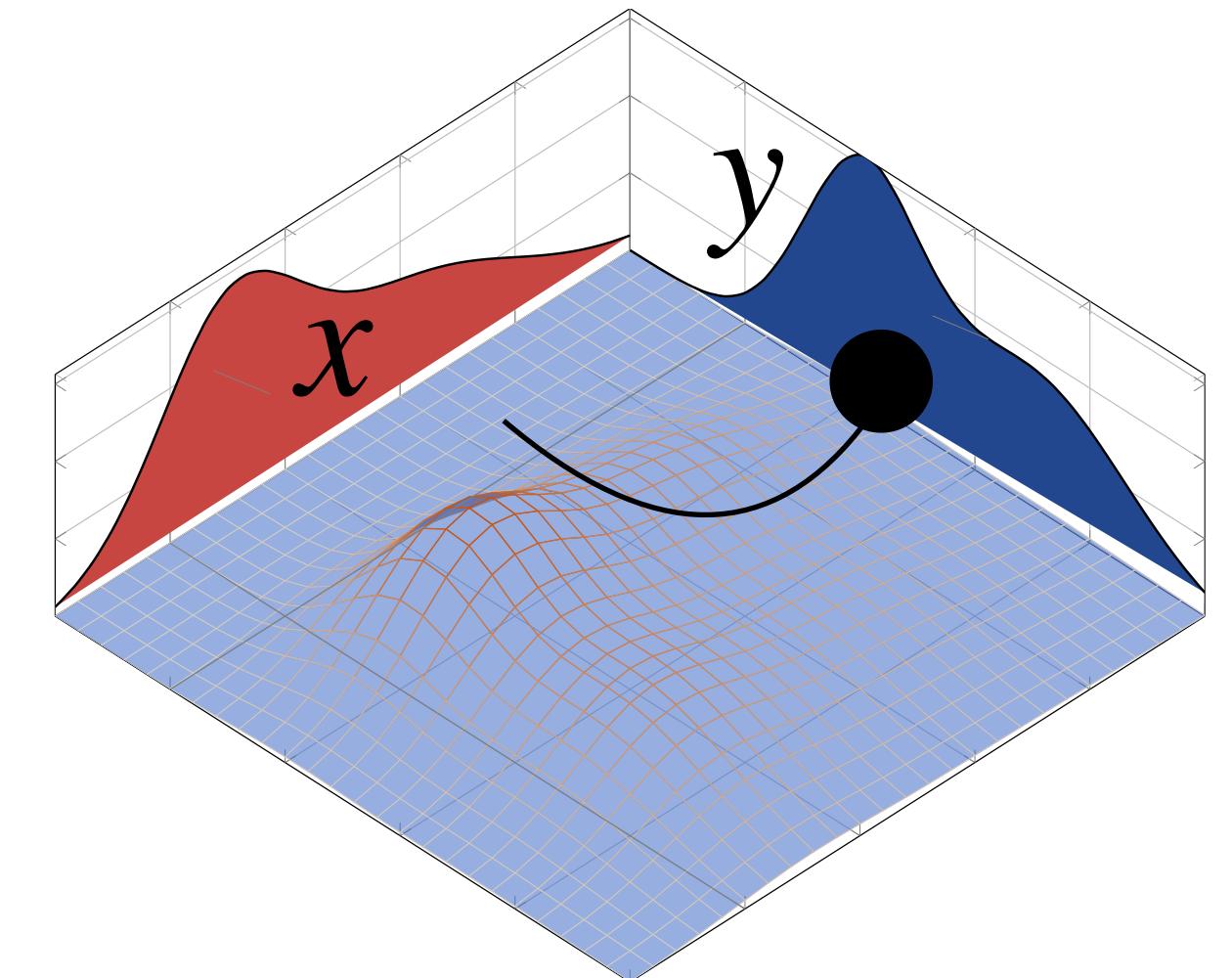
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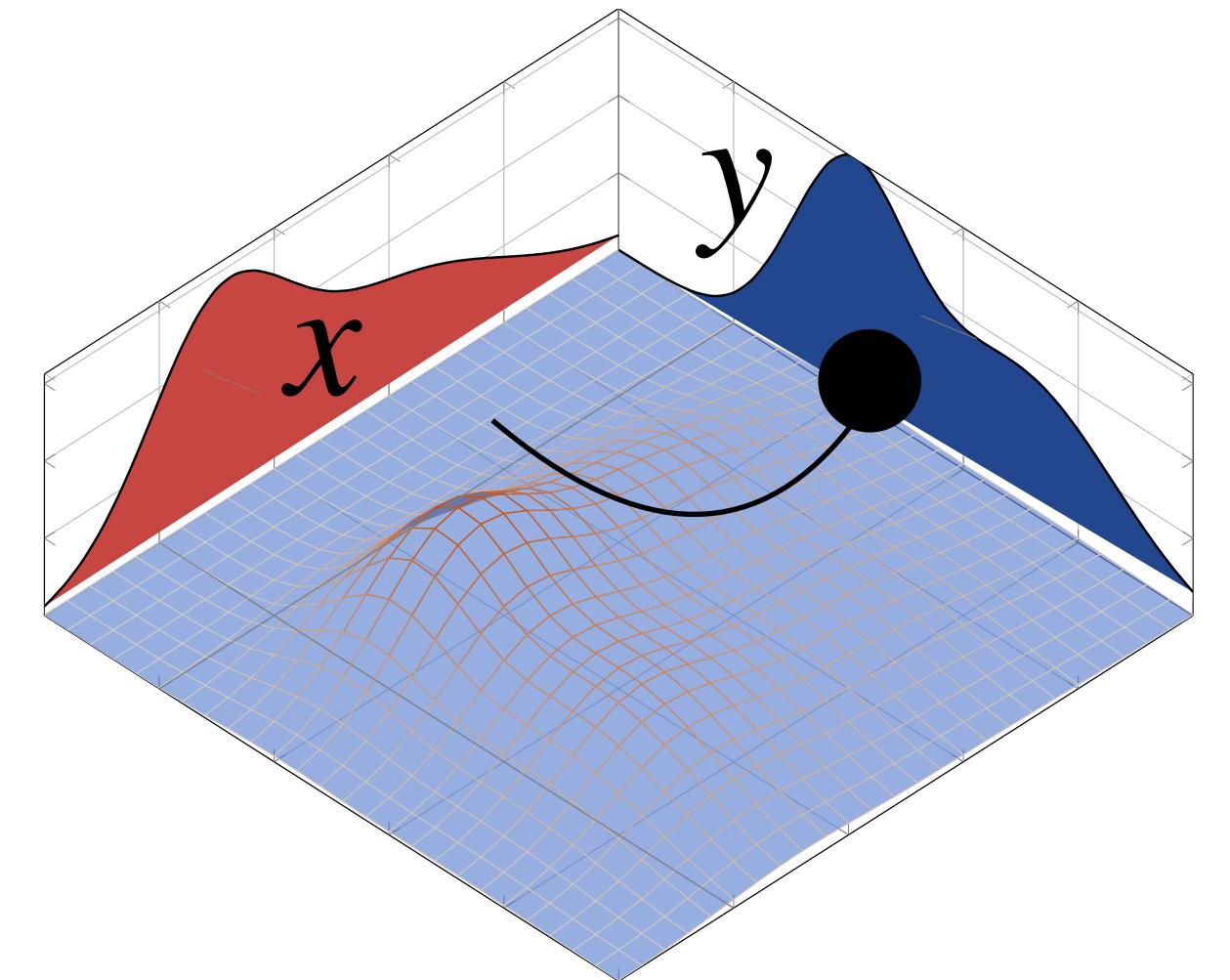
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$$= \sup \left\{ \int \psi_1(x) dP(x) + \int \psi_2(y) dQ(y) \mid \psi_1(x) + \psi_2(y) \leq |x - y|^p \right\}$$

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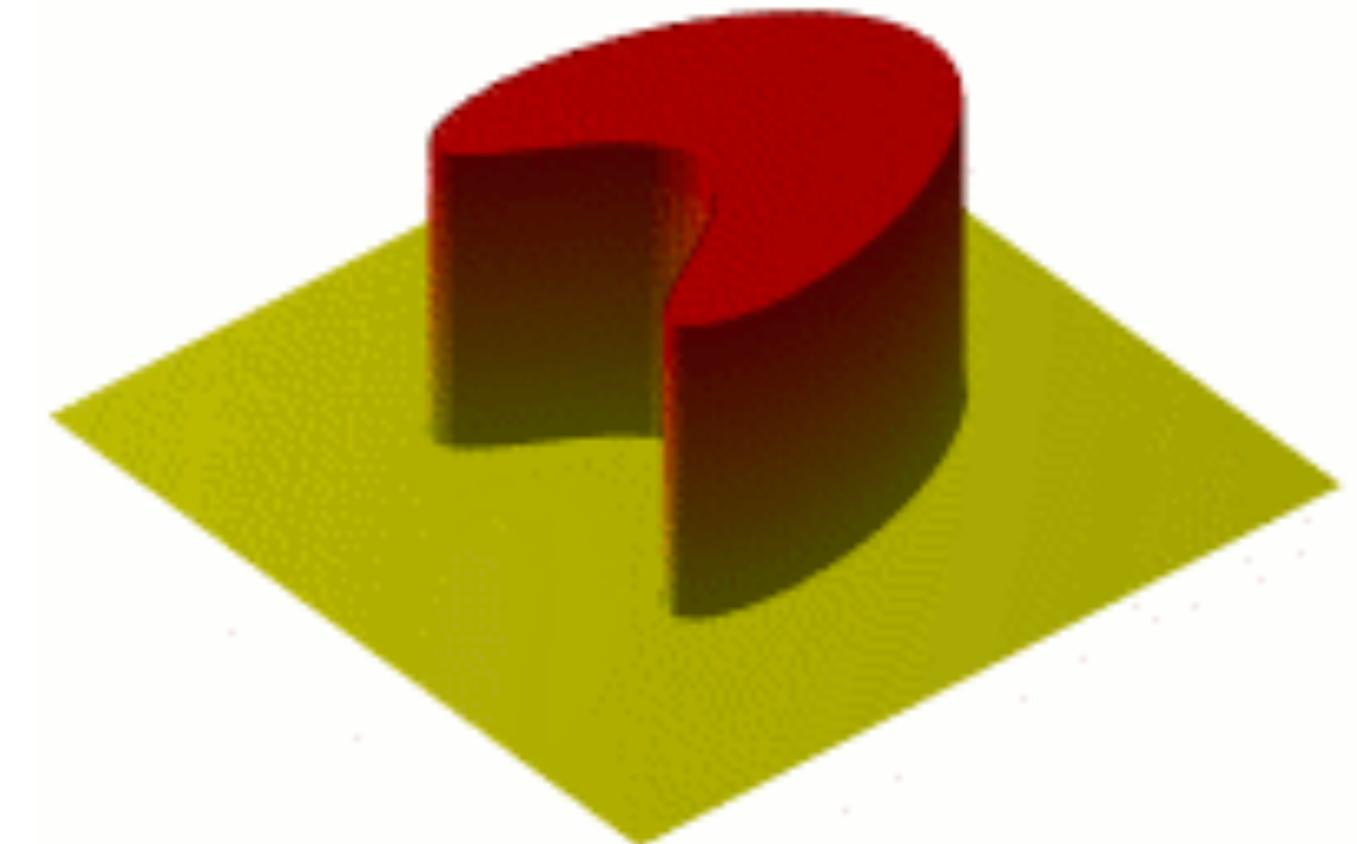
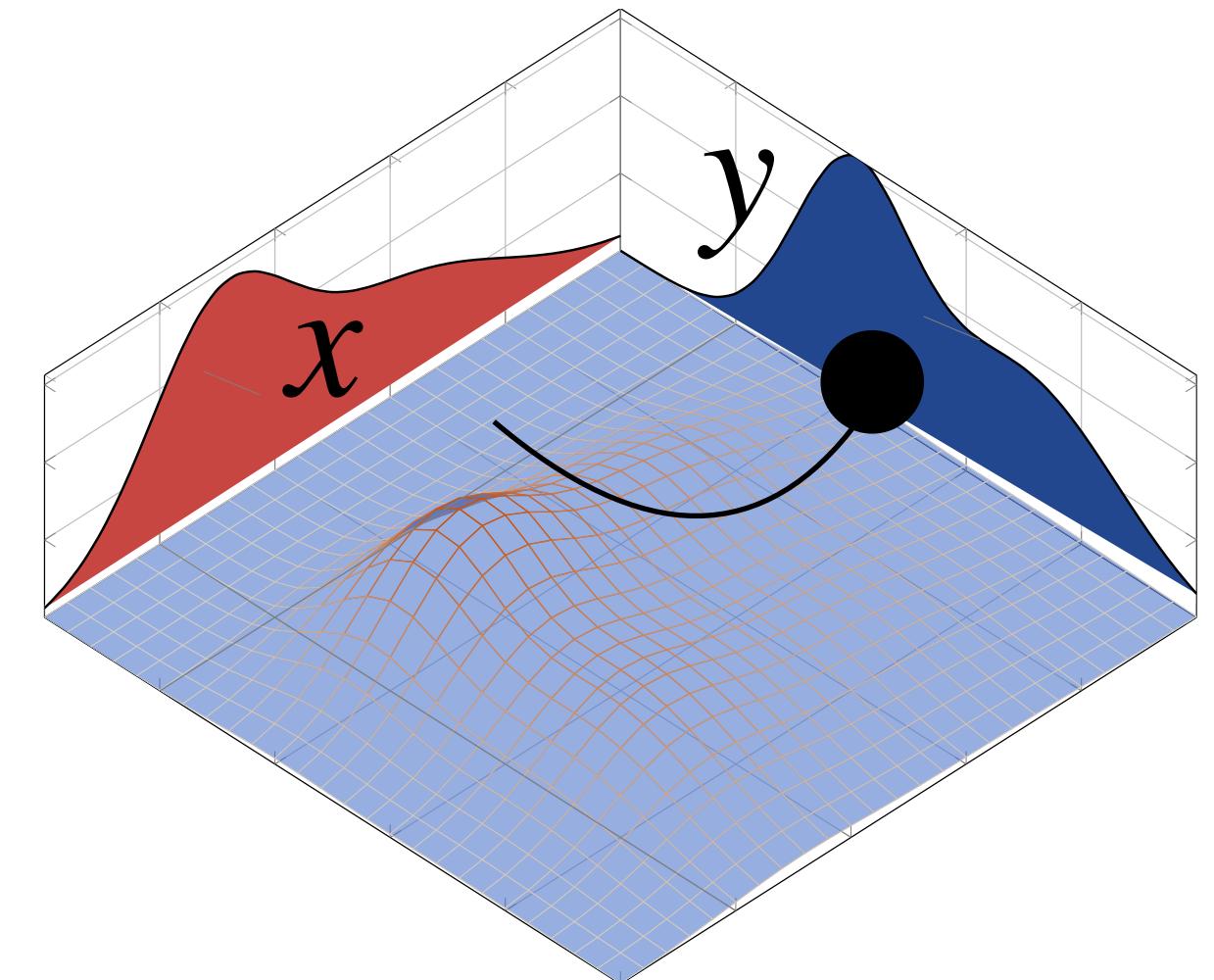
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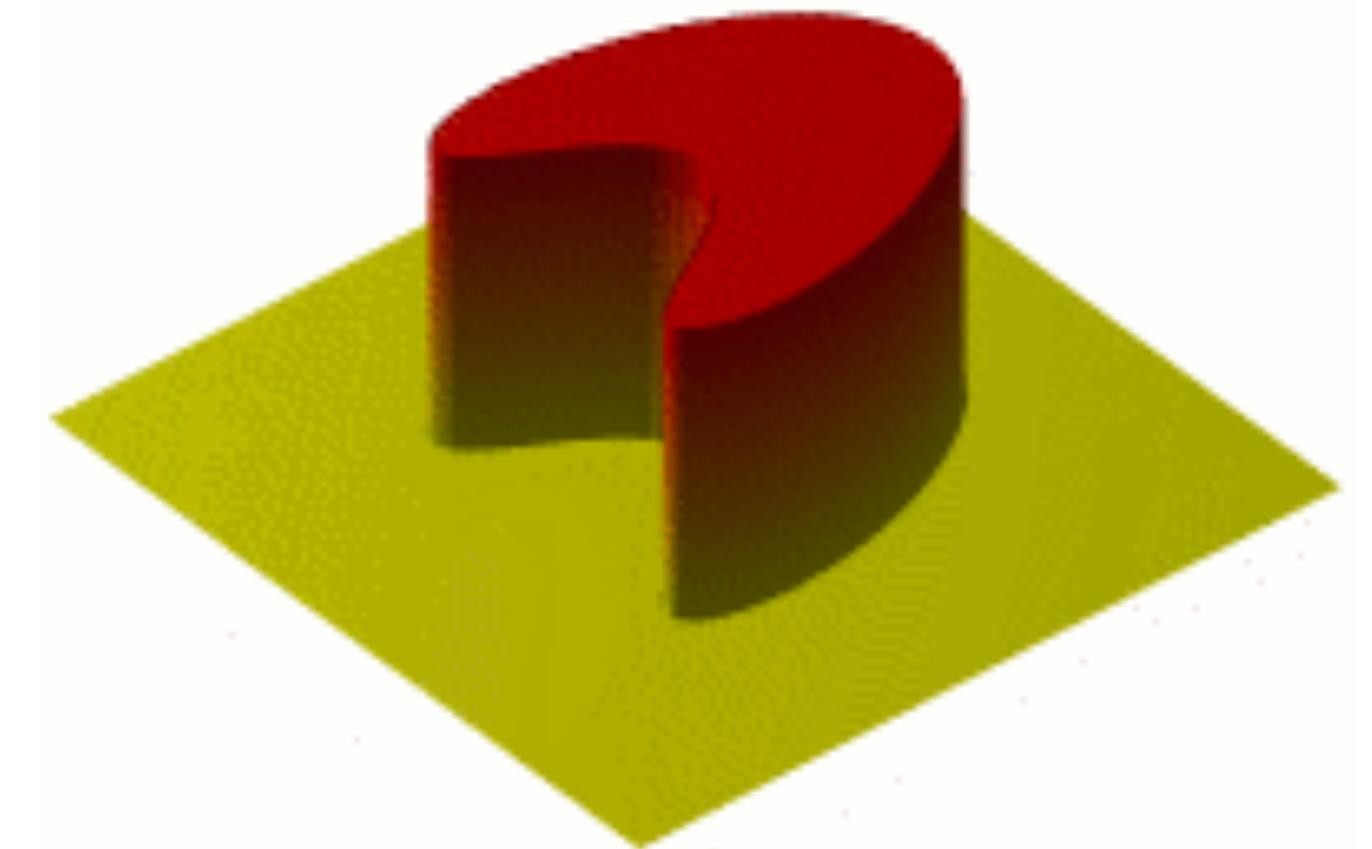
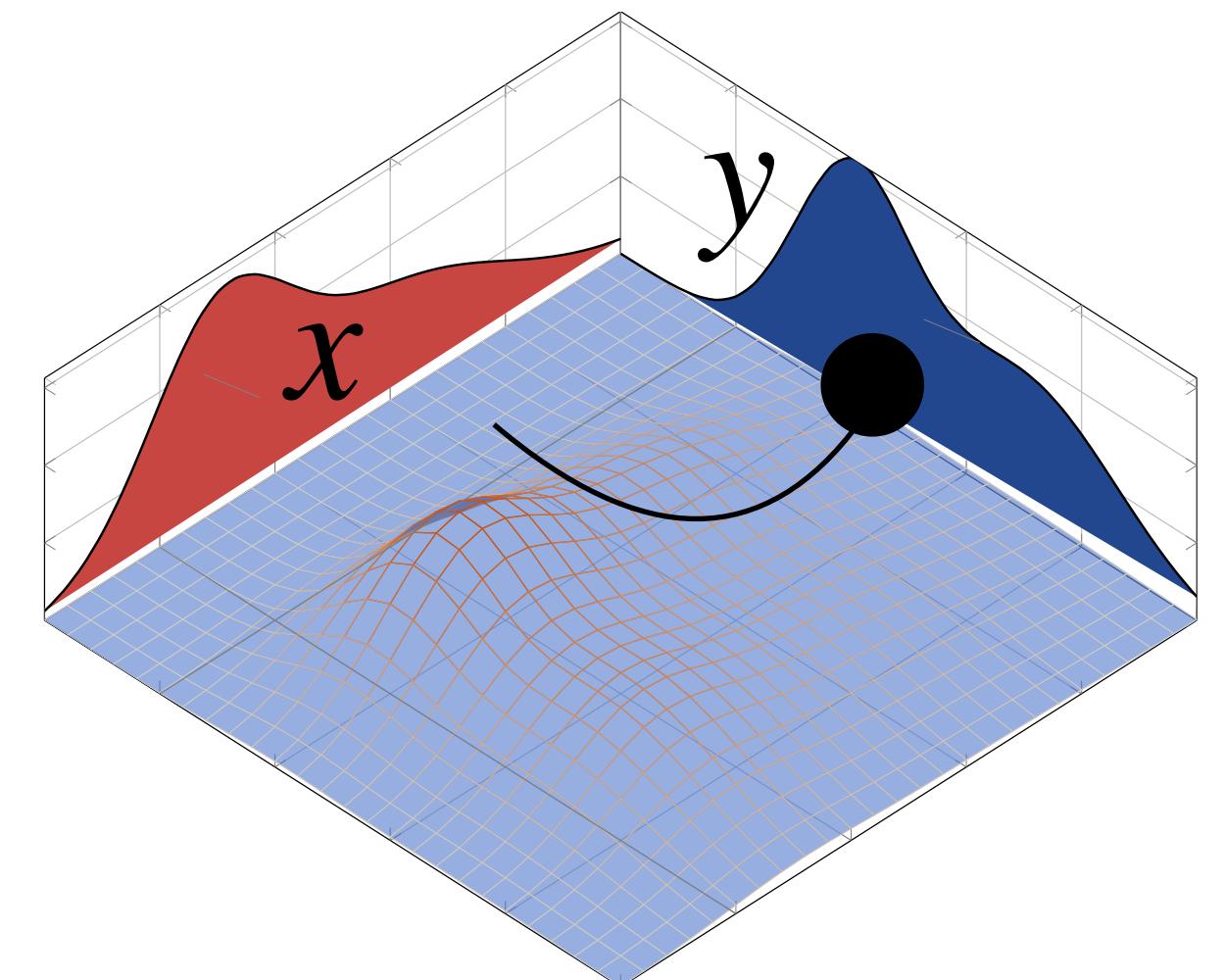
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Example. Entropy-OT [Cuturi 2013] Duality leads to faster computation

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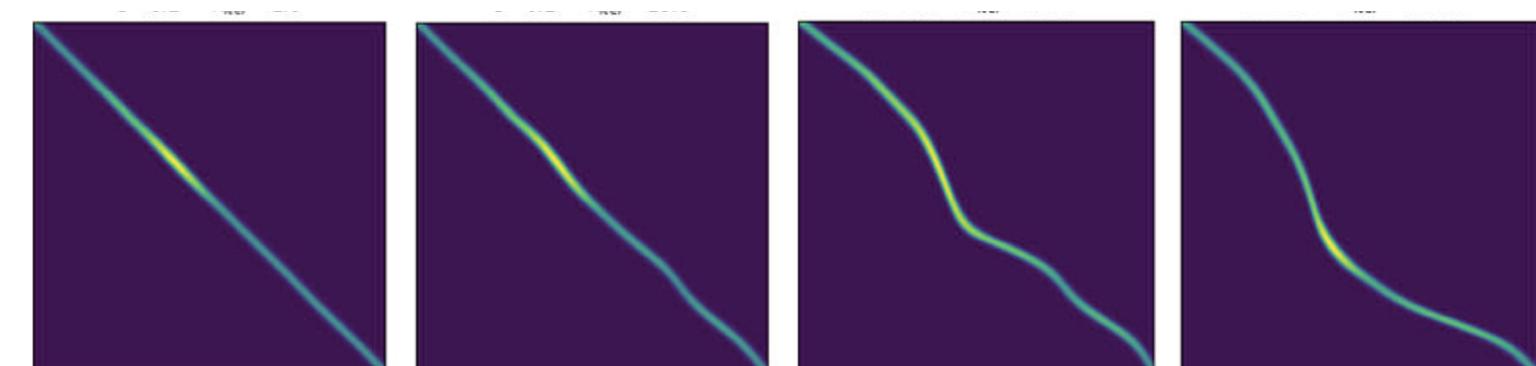
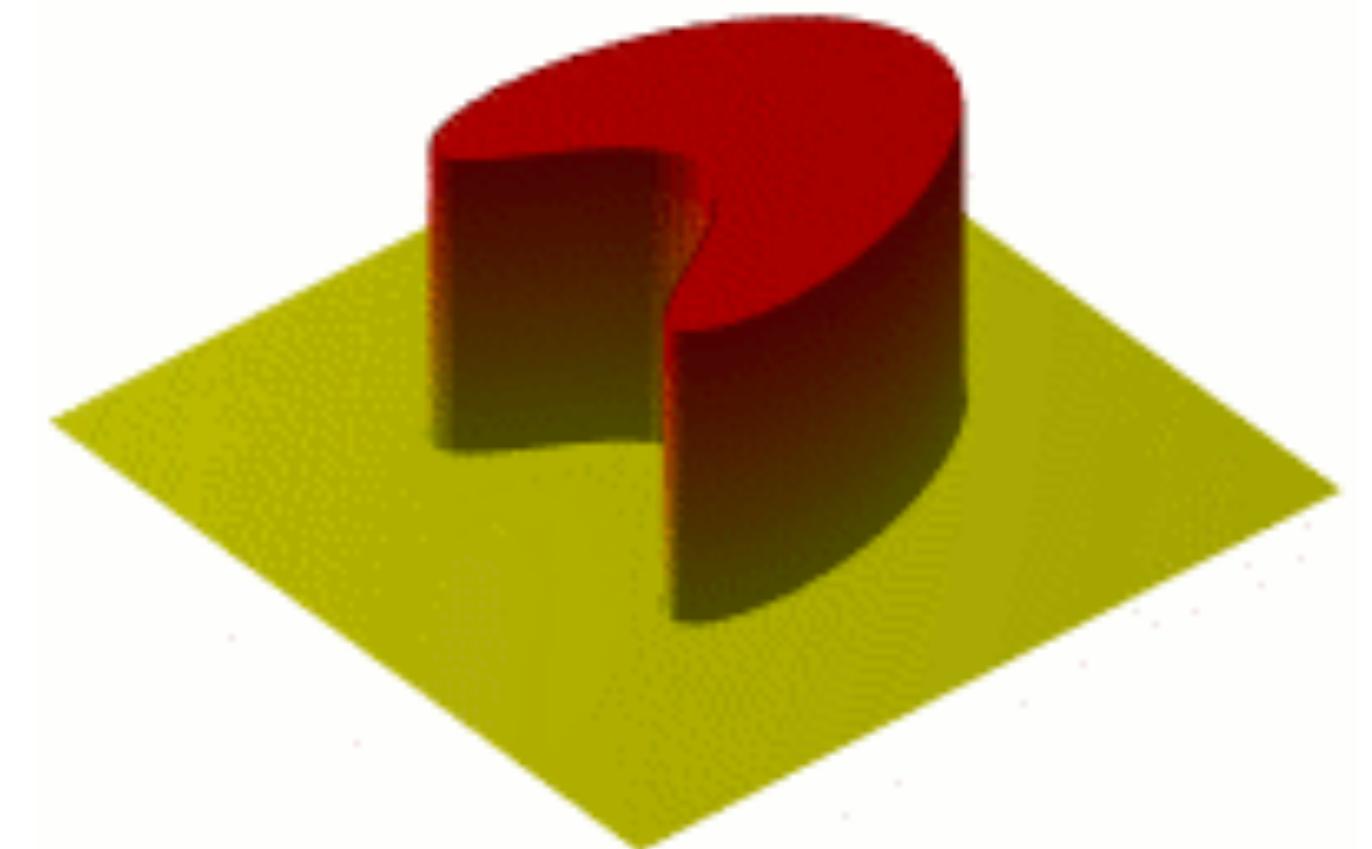
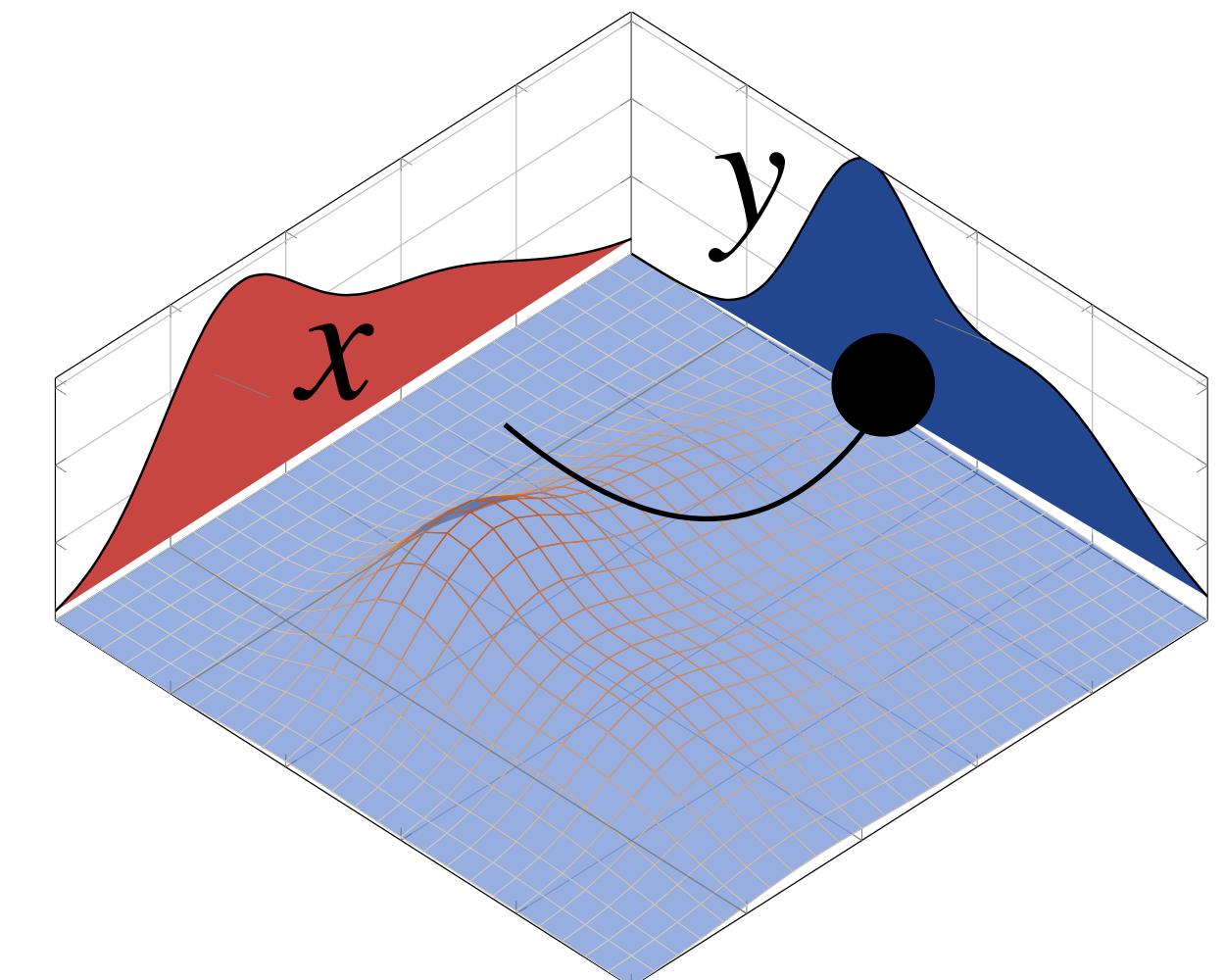


Figure credit: Wiki., M. Cuturi, A. Genevay

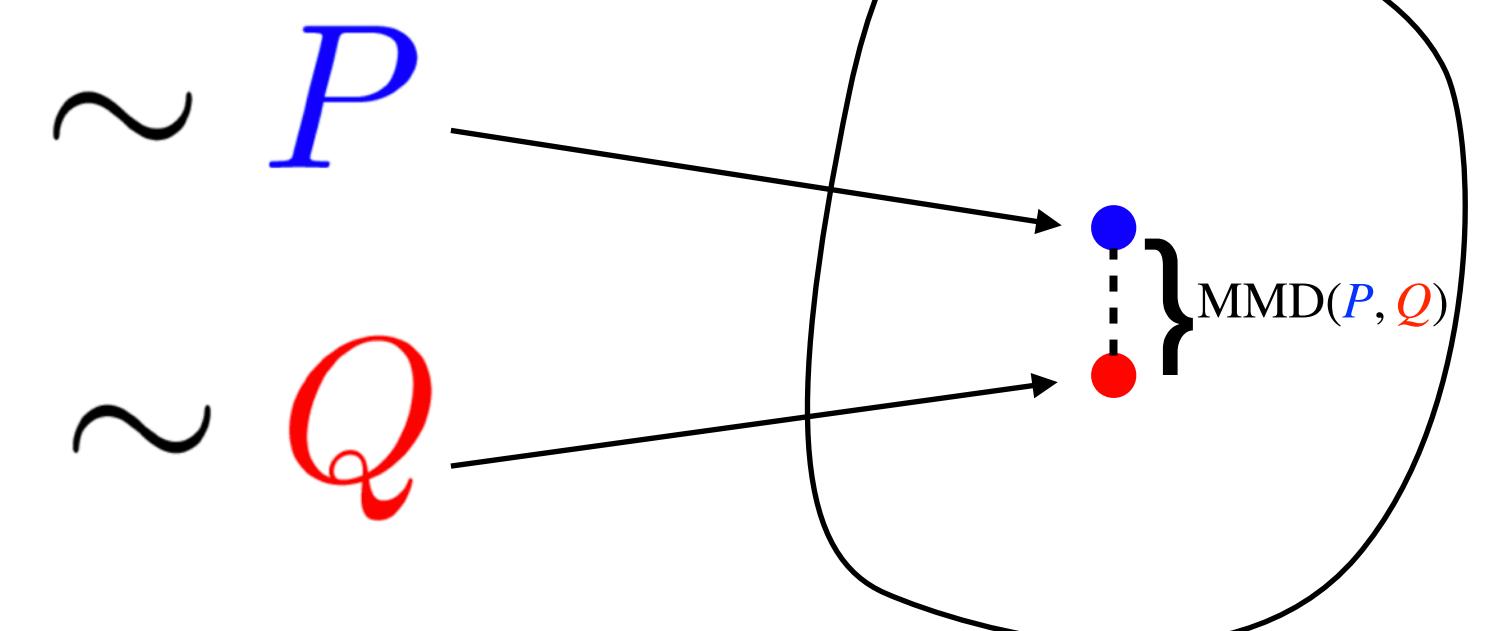
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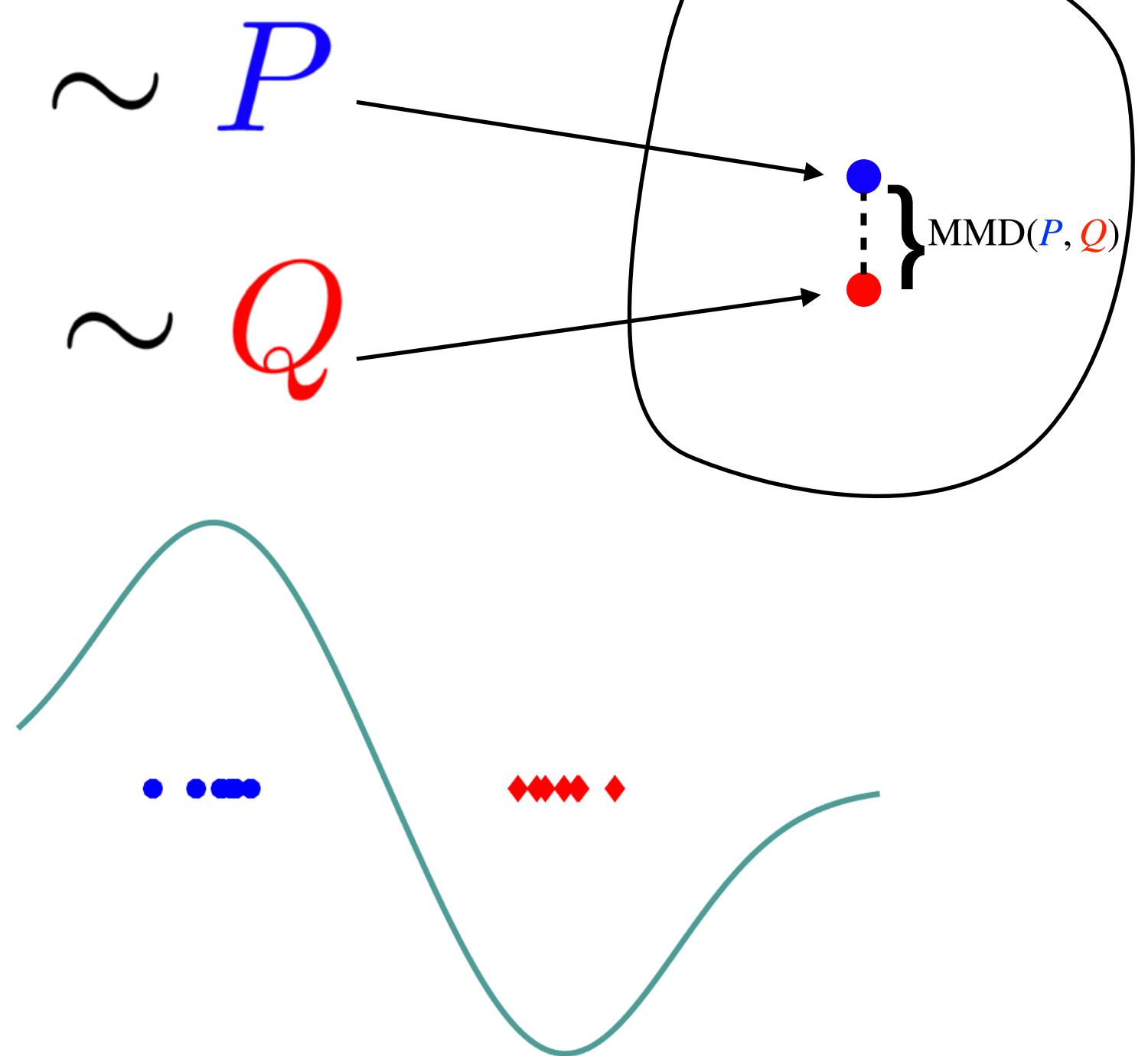
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Dual formulation as an integral probability metric.

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

\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} .



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

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

Dual formulation as an integral probability metric.

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

\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. Entropy-MMD [Kremer et al. 2023]

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

Duality leads to “interior point method” for prob. distributions

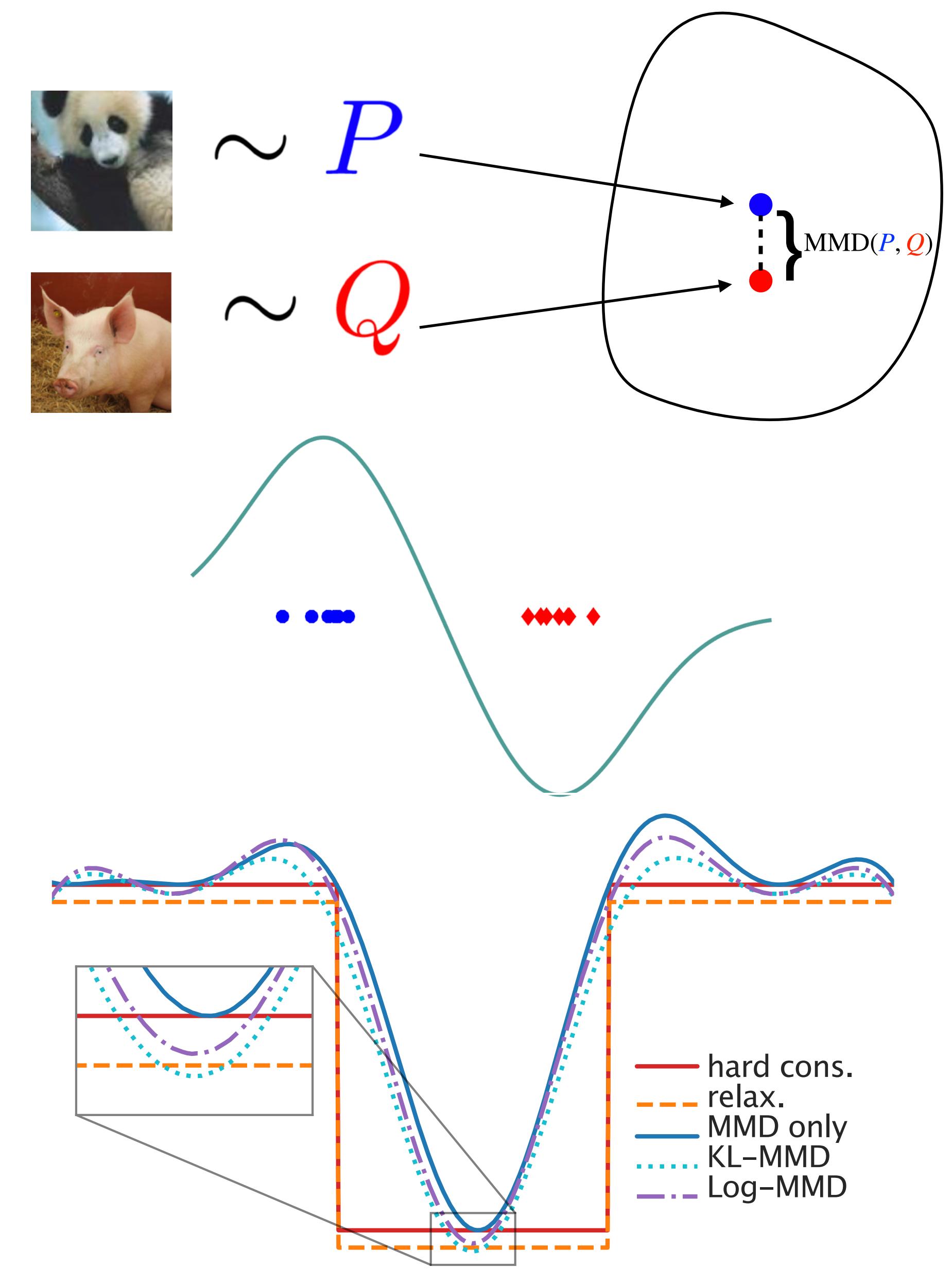


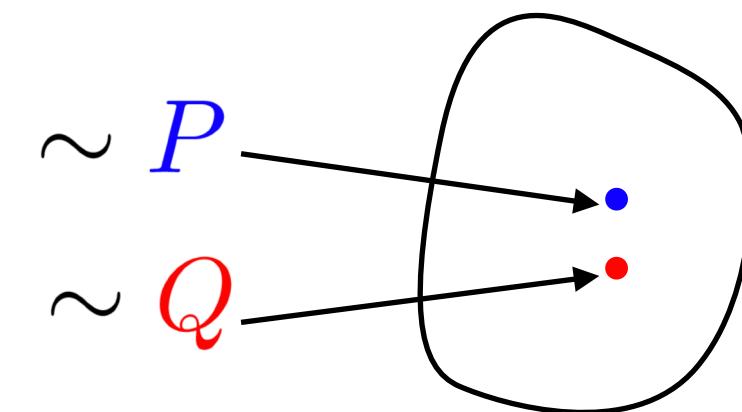
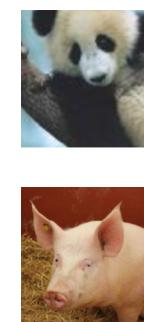
Figure credit: W. Jitkrittum, J. Zhu, H. Kremer

Previous work: Kernel DRO

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Primal DRO (not solvable as it is)

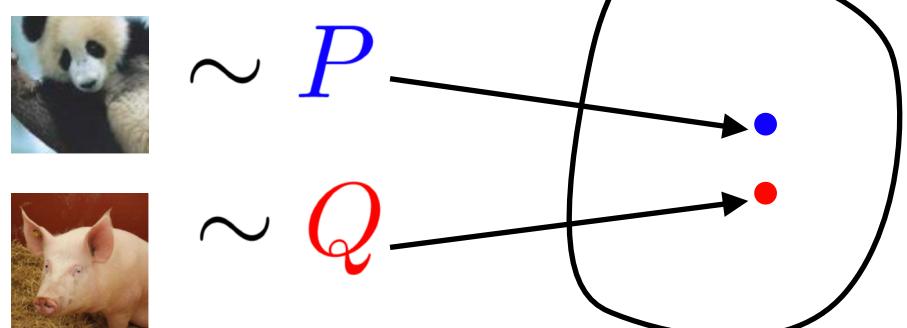
$$(\text{DRO}) \quad \min_{\theta} \quad \sup_{\substack{\mathbb{E}_{\mathcal{Q}} l(\theta, \xi) \\ \text{MMD}(\mathcal{Q}, \hat{P}) \leq \epsilon}} \mathbb{E}_{\mathcal{Q}} l(\theta, \xi)$$



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Kernel DRO Theorem (simplified). [Z. et al. 2021]

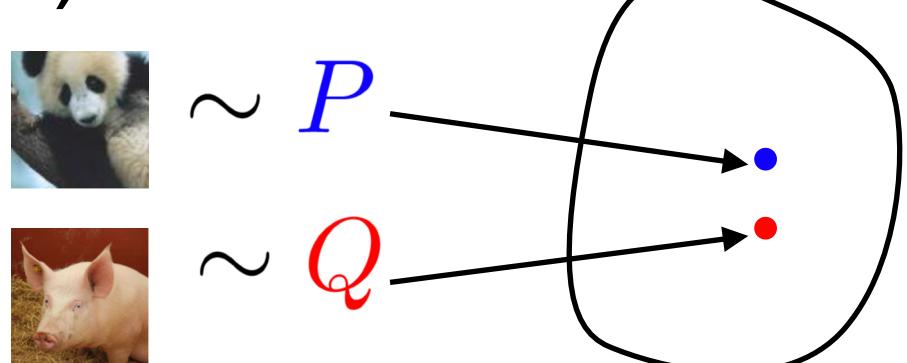
DRO problem is equivalent to the dual kernel machine learning problem, i.e., (DRO)=(K).

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

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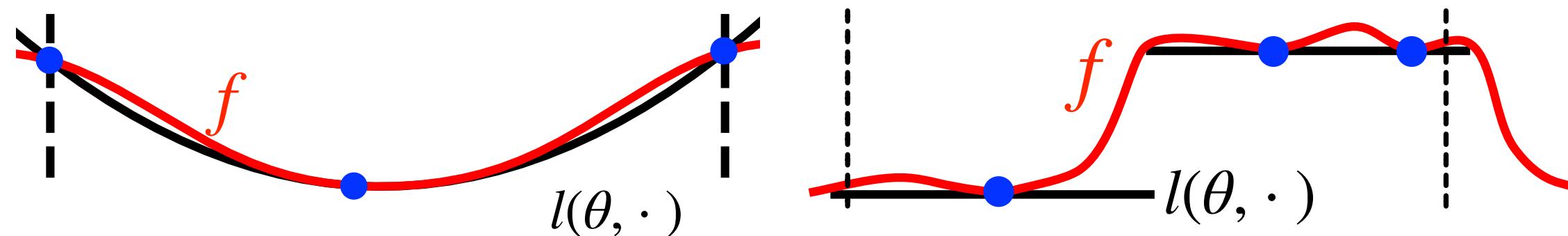


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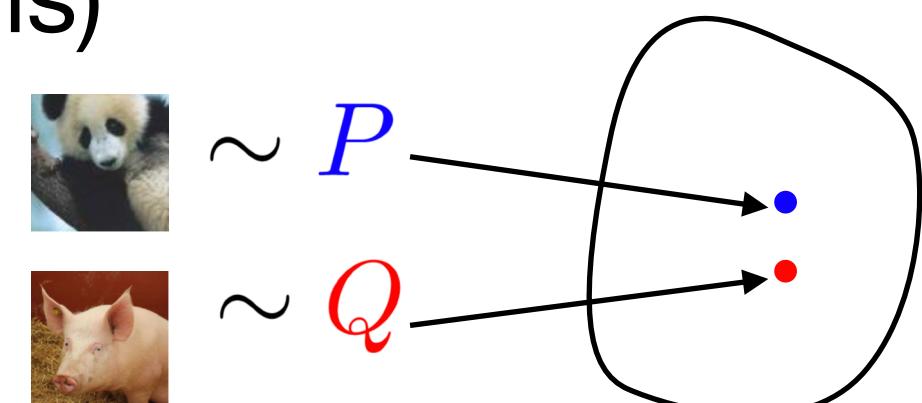
Geometric intuition: **dual kernel function f** as robust surrogate losses (flatten the curve)



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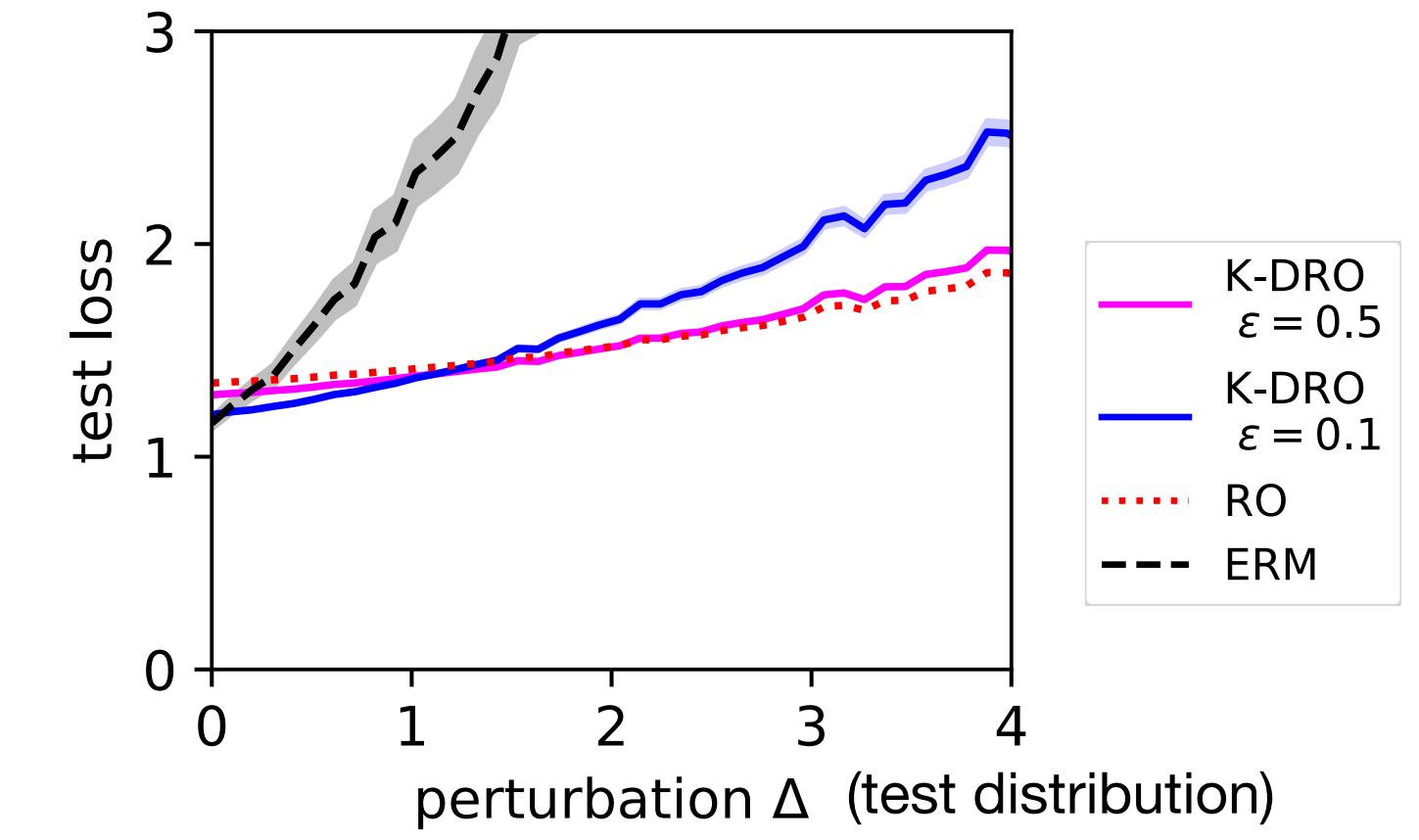
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Example. Robust least squares

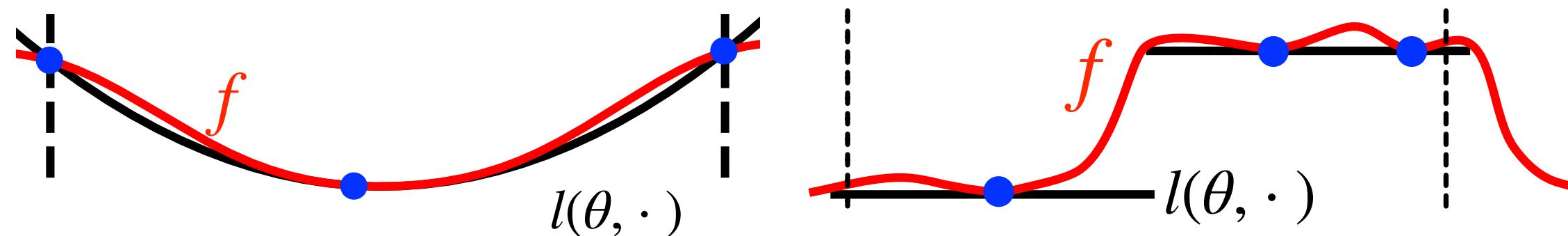
[El Ghaoui Lebret '97]

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

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



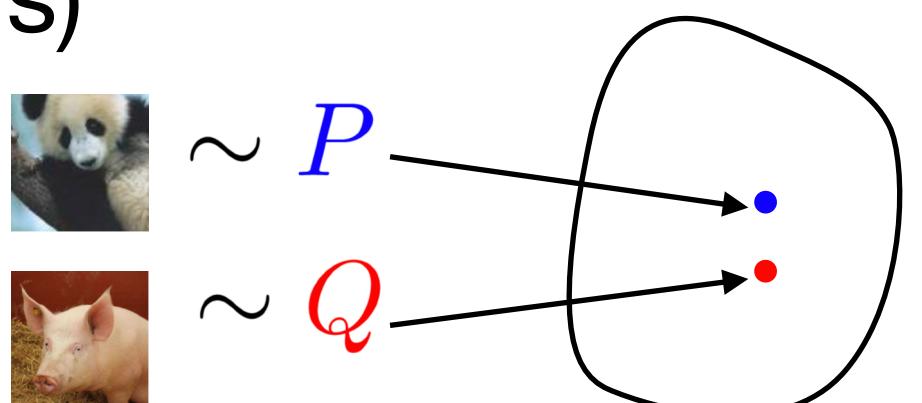
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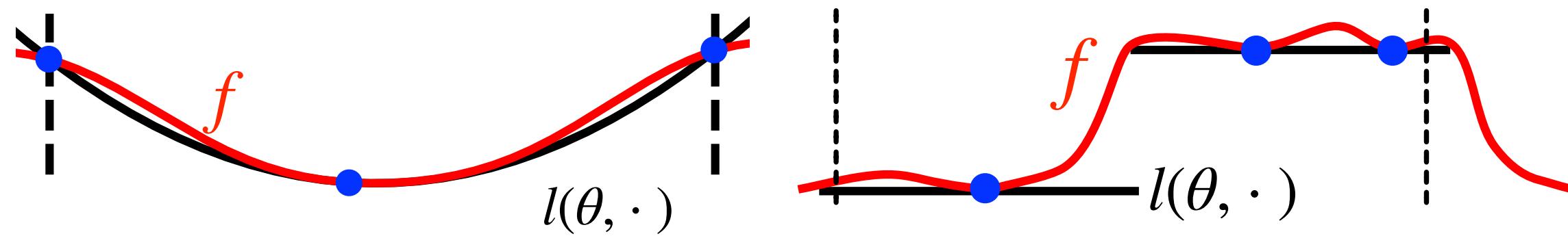


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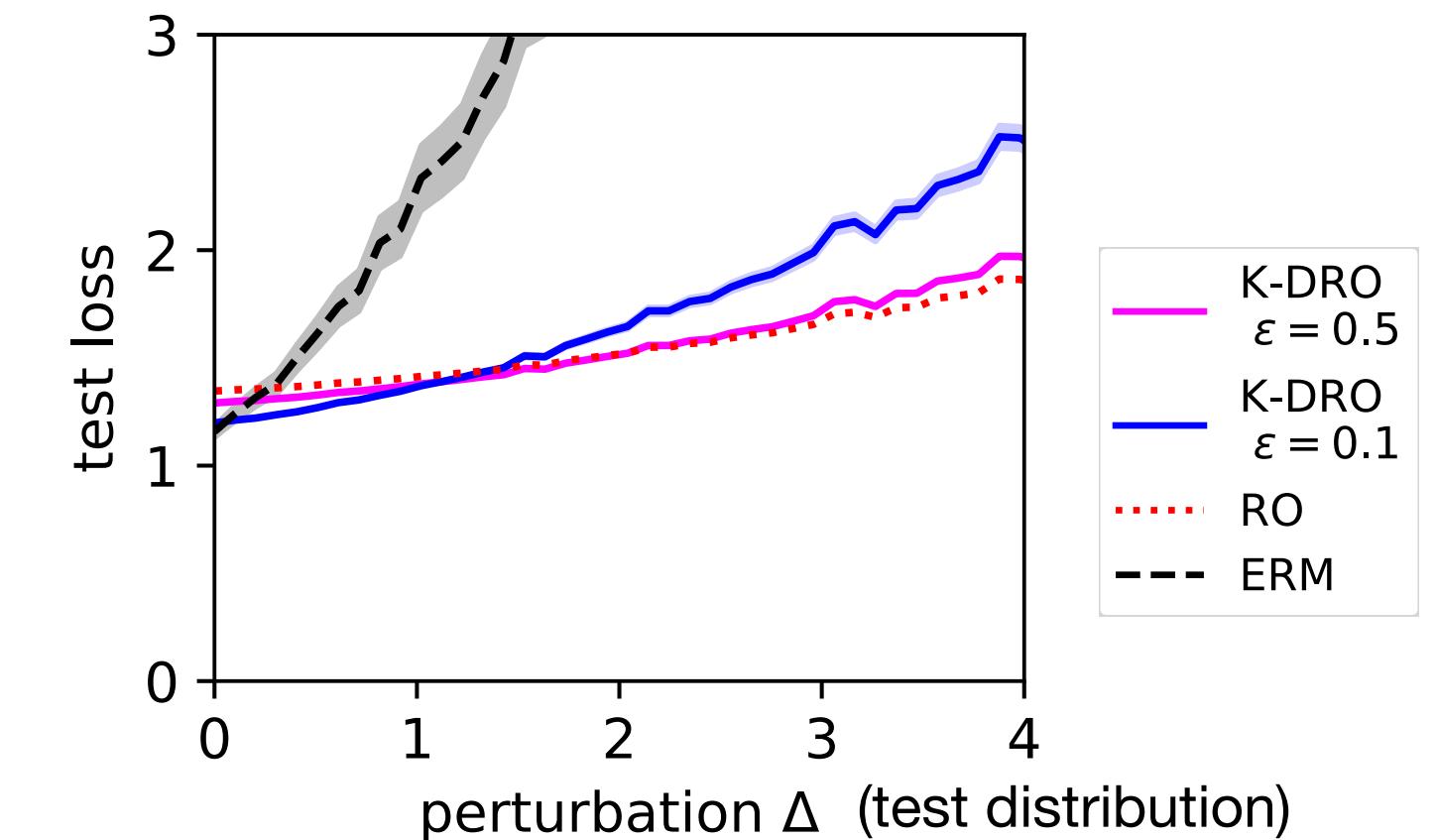


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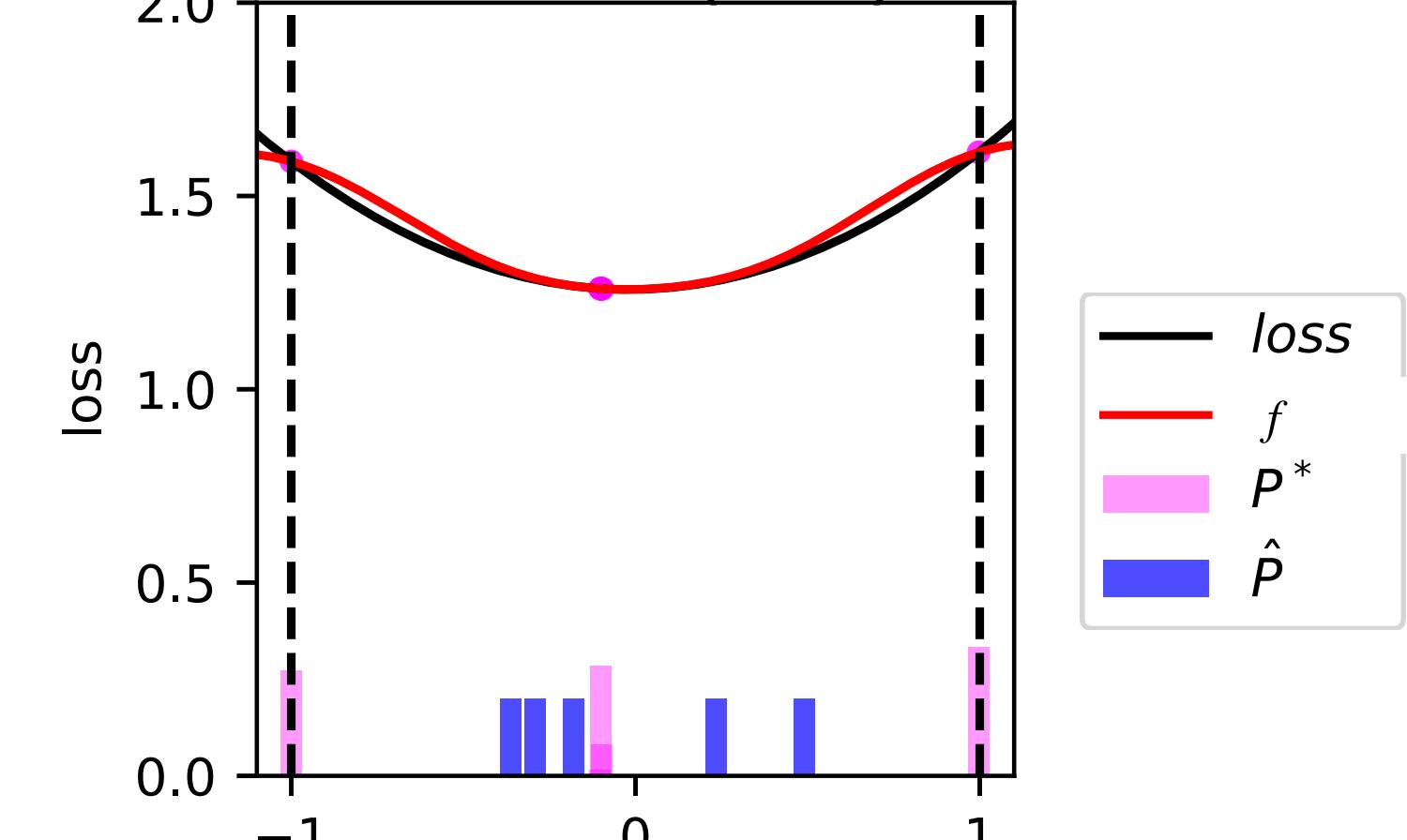
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Robustifying with DRO

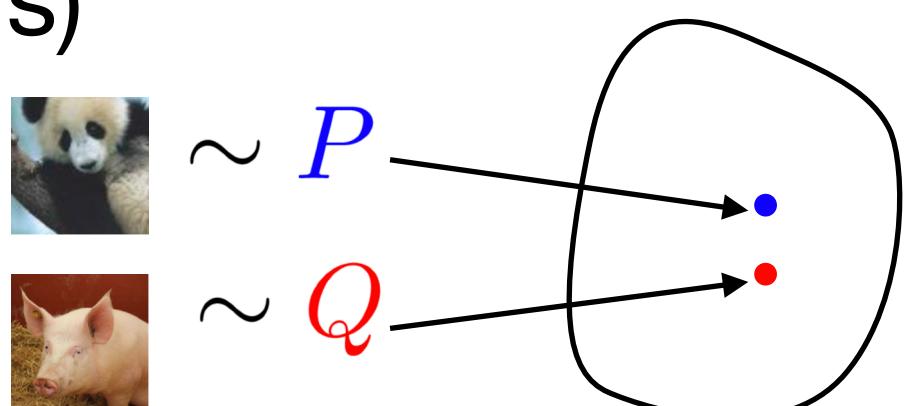
f as witness (test) function



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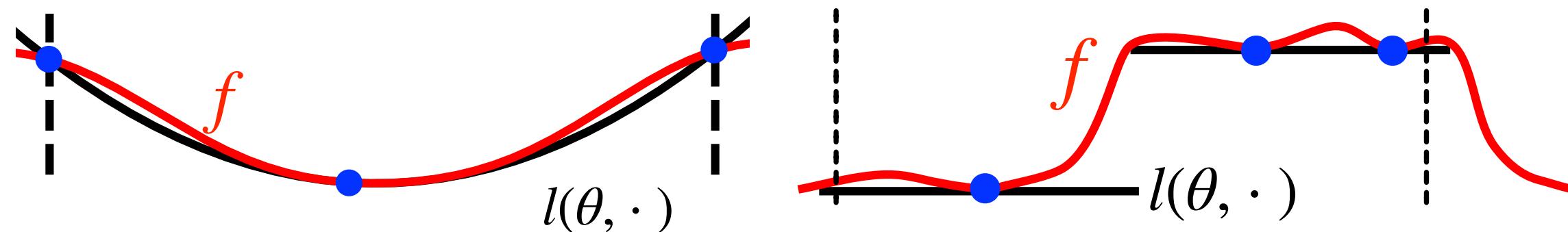


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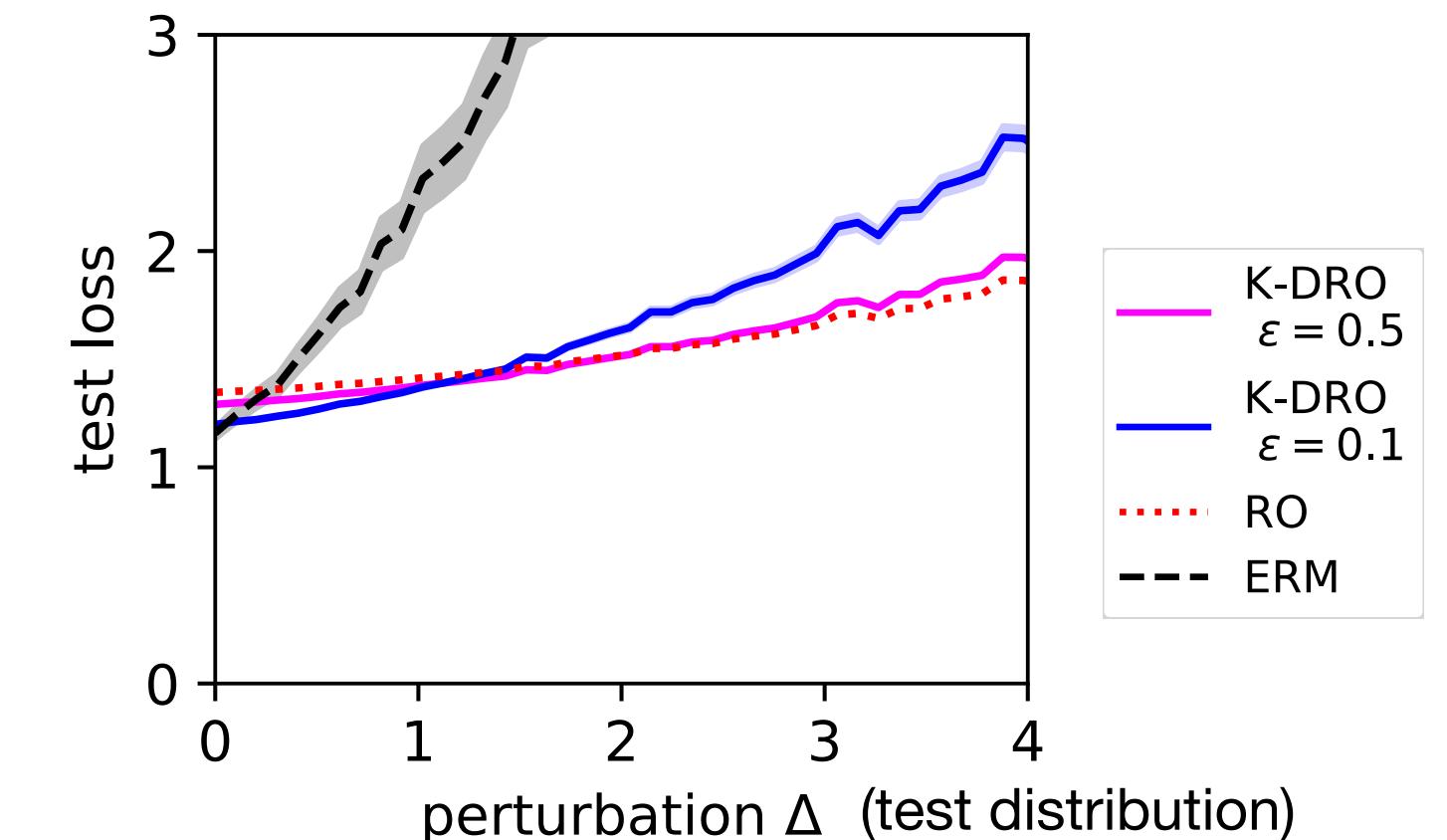


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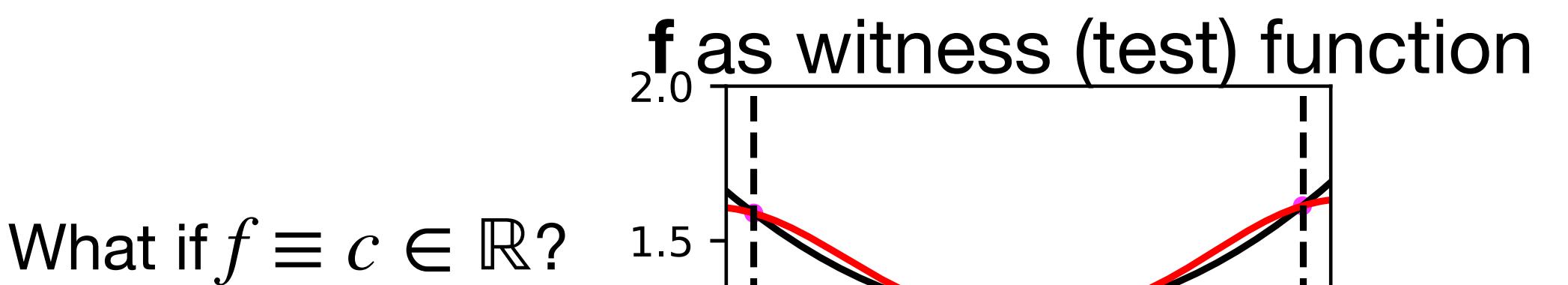
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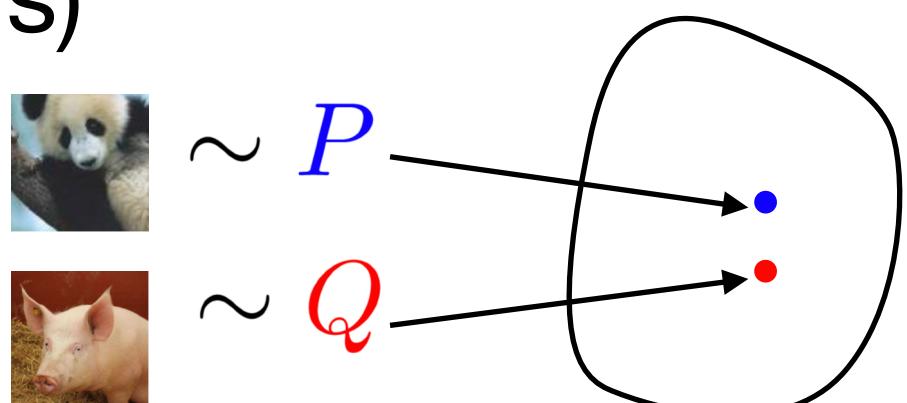


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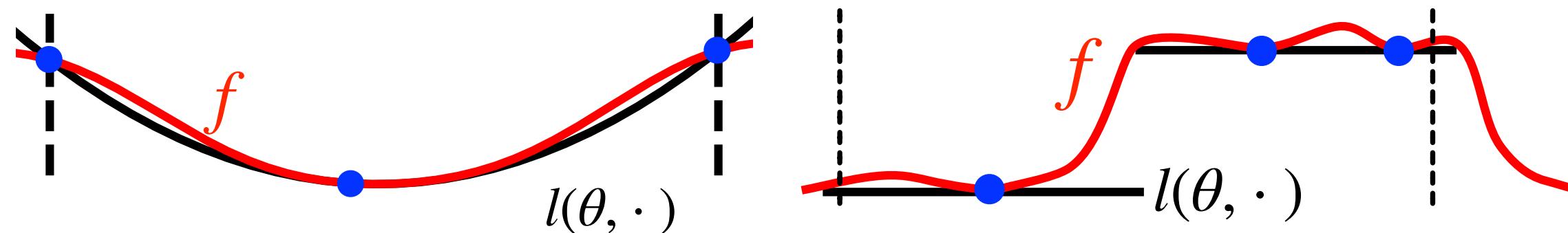


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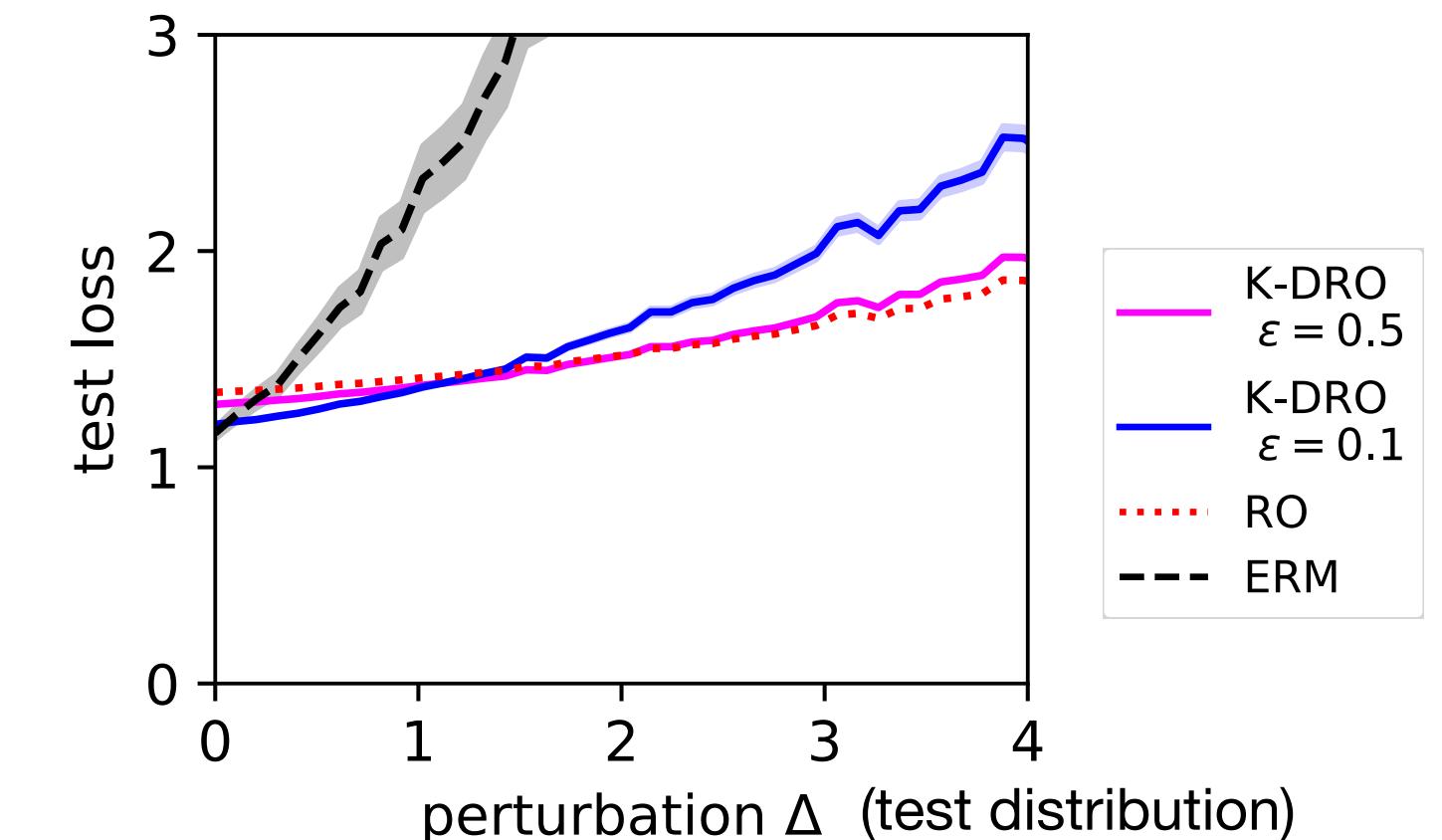


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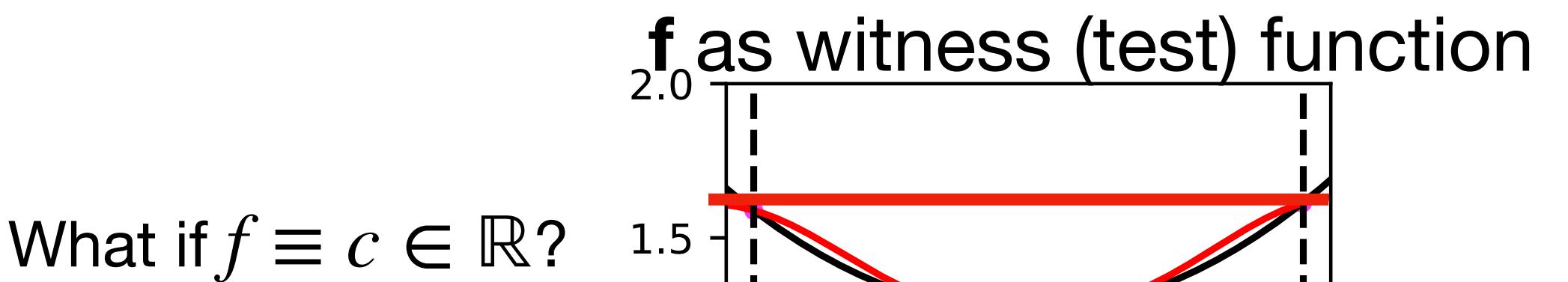
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Duality perspective

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2-Wasserstein

Kernel DRO [z. et al. 2021]

Primal:

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Dual:

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where Moreau envelope

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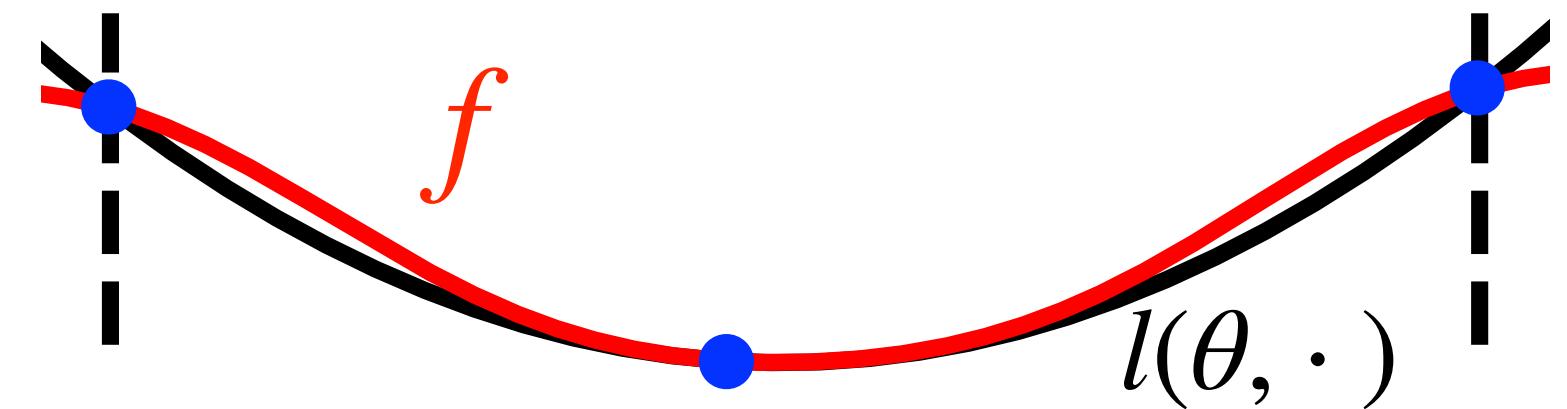
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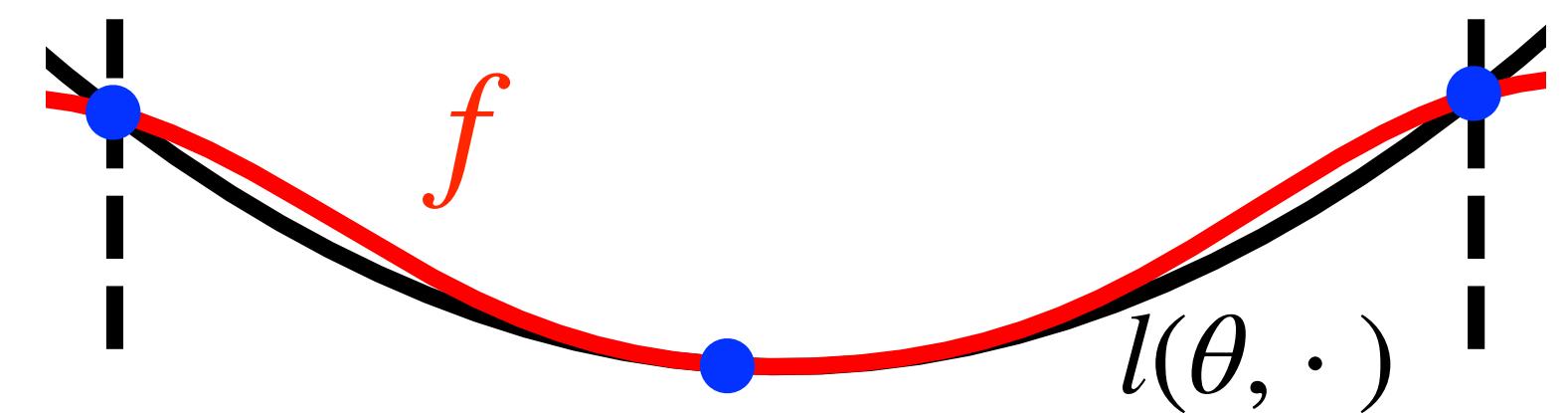
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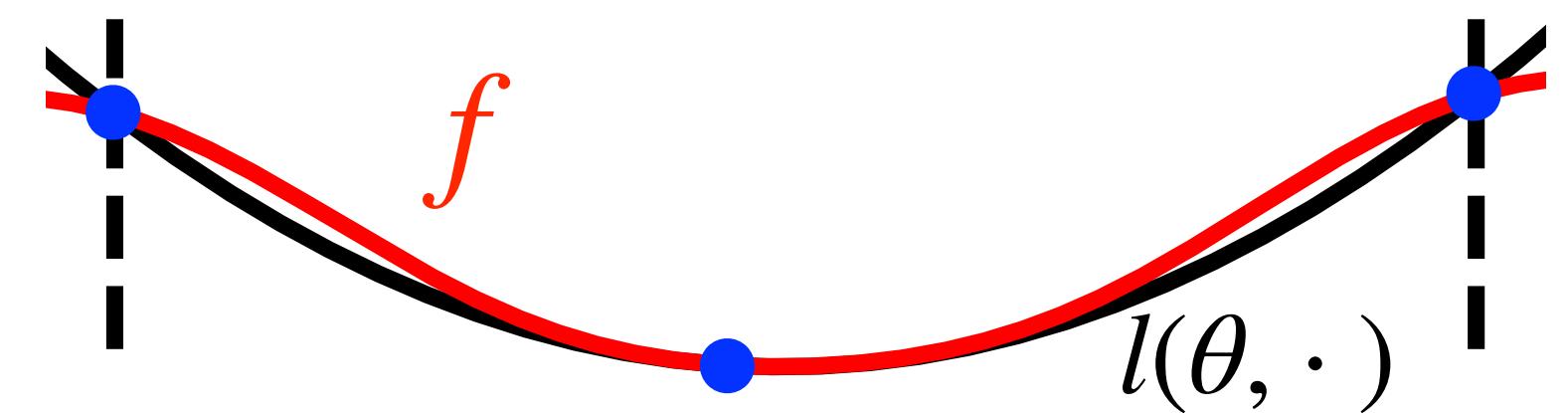
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Nonlinear kernel approx. as robust surrogate losses (flatten the curve)

Dynamic: Duality of Gradient Flow

From static DRO to JKO scheme for gradient flows

DRO's Wasserstein measure optimization is not new.

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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 .

Duality in gradient flow dynamics: nonlinear ODE

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If $X \not\cong X^*$: $\dot{u} \in \partial R^*(\mu, -DF) \subset T_u M$ (**rate**) **vs** $0 \in DF + \partial R(\mu, \dot{\mu}) \subset T_u^* M$ (**force**)

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

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

Duality in the Wasserstein gradient flow

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

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

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

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

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Duality in the Wasserstein gradient flow

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

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

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

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

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Compared with the Wasserstein GF of entropy, our kernel 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]

$$\min_{\theta} \sup_{\substack{\mathbb{E}_P I(\theta, \xi), \\ \text{MMD}(P, \hat{P}) \leq \epsilon}} \mathbb{E}_P I(\theta, \xi),$$

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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 $\nabla I(\theta, \xi)$. (see also an alternative using kernel mirror prox. [Dvurechensky & Zhu])

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