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 in ML

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

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

Wasserstein barycenter

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

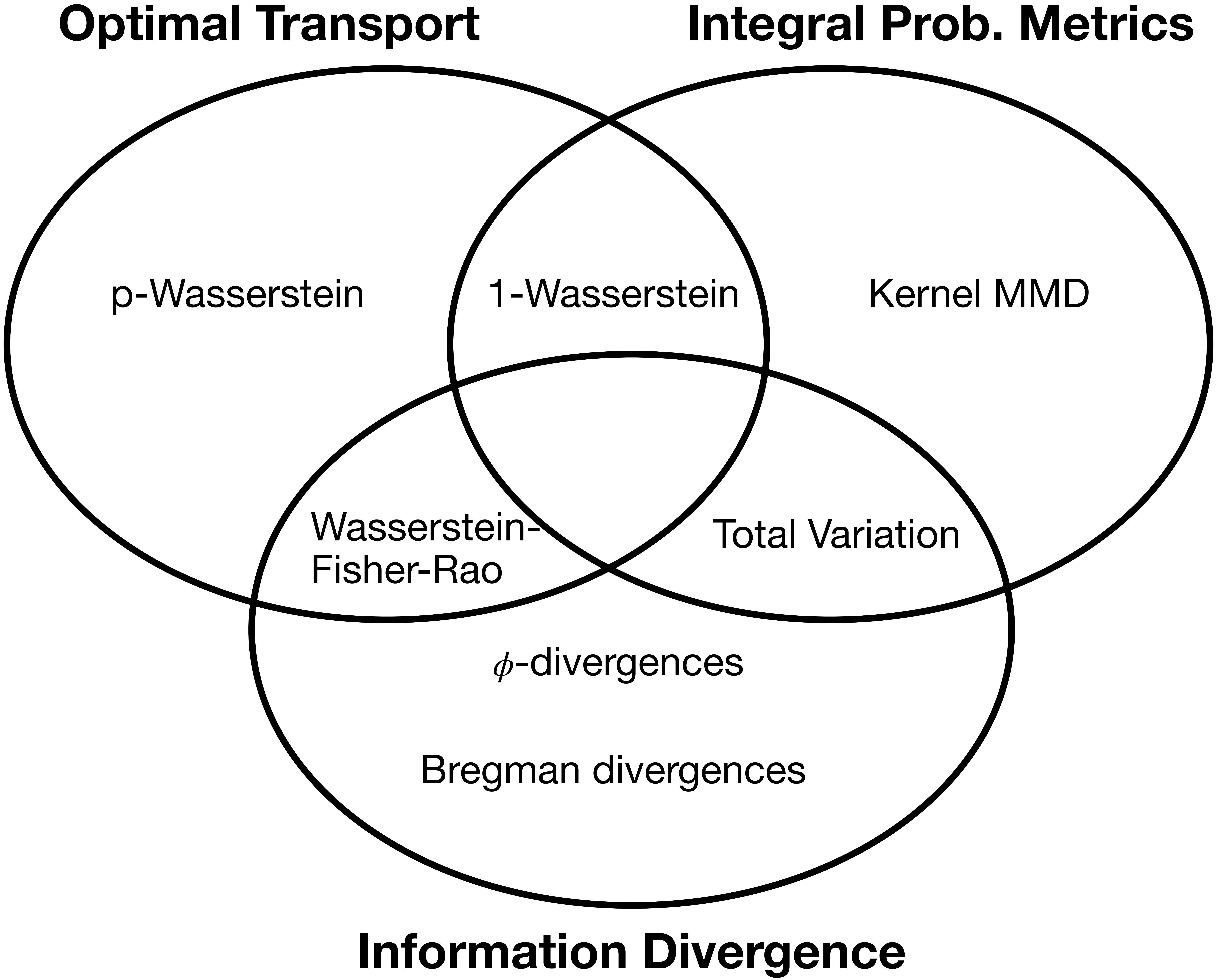
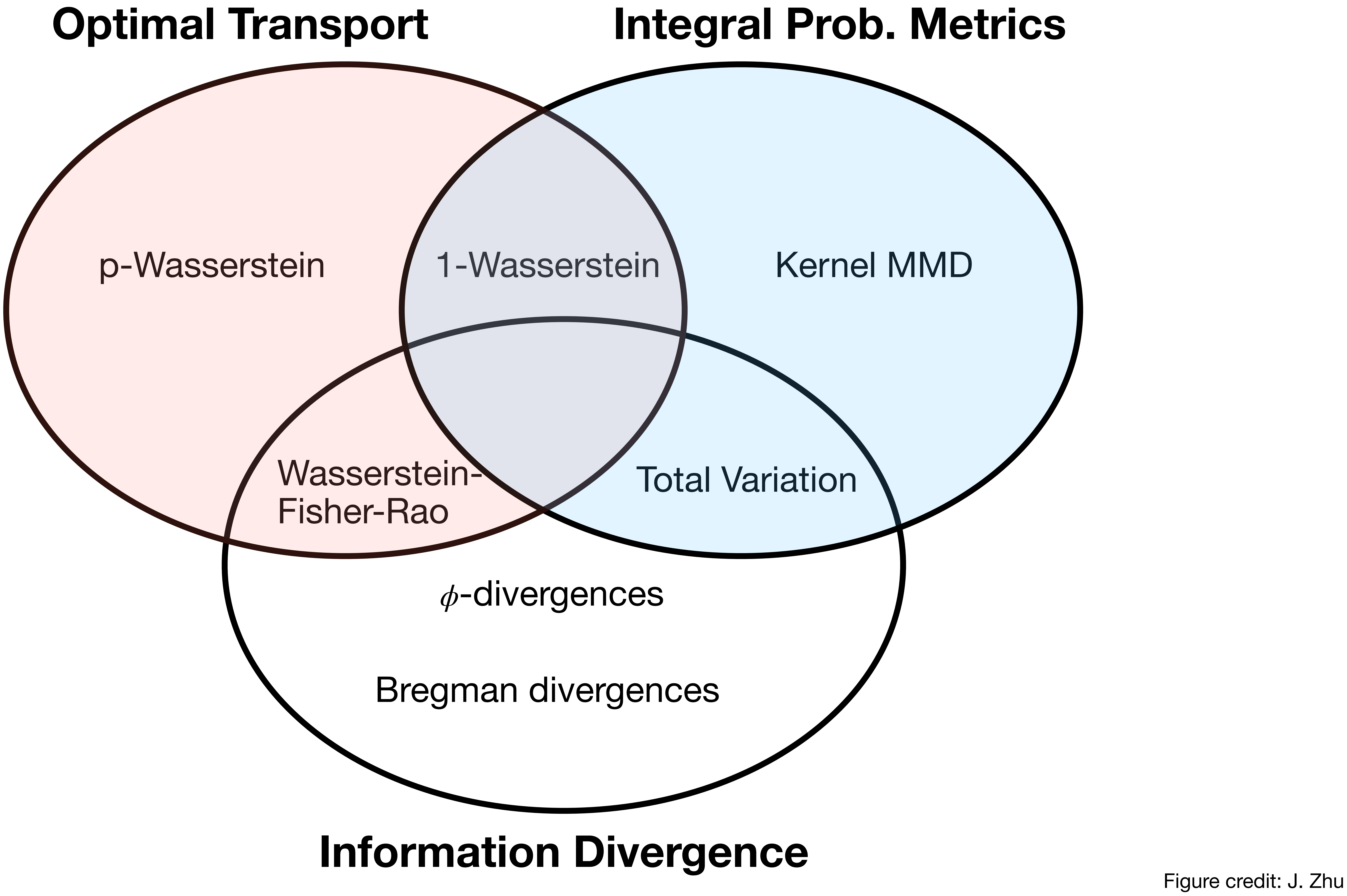


Figure credit: J. Zhu


Optimal Transport
Integral Prob. Metrics
p-Wasserstein
1-Wasserstein
Kernel MMD
Wasserstein-
Fisher-Rao
Total Variation
ϕ-divergences
Bregman divergences
Information Divergence
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Static: Duality of Distributionally Robust Learning

Distributional robustness, but what kind?

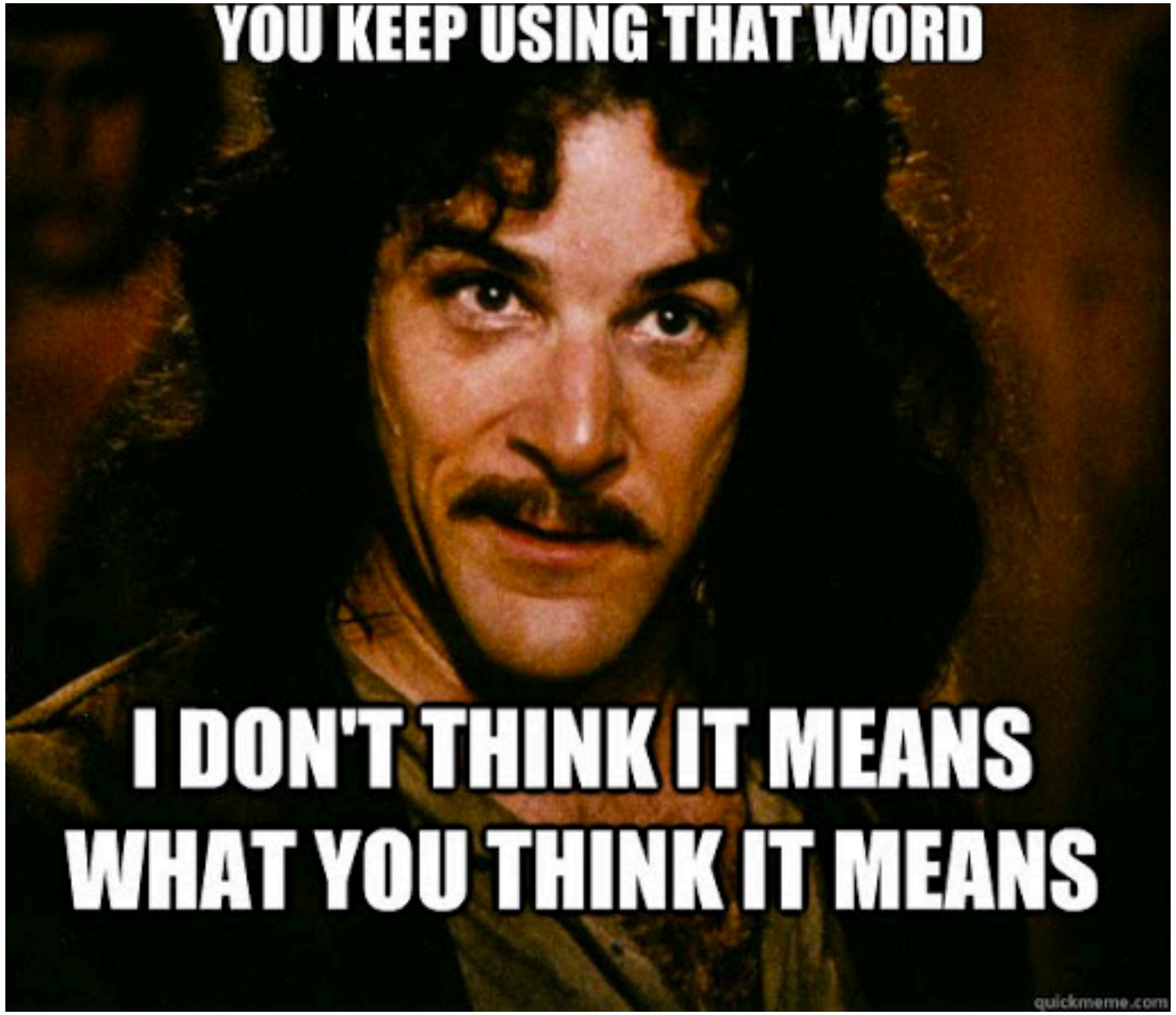

Figure credit: The Princess Bride,
a bedside story by your grandpa

From Statistical Learning to Distributionally Robust Learning

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Empirical Risk Minimization

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

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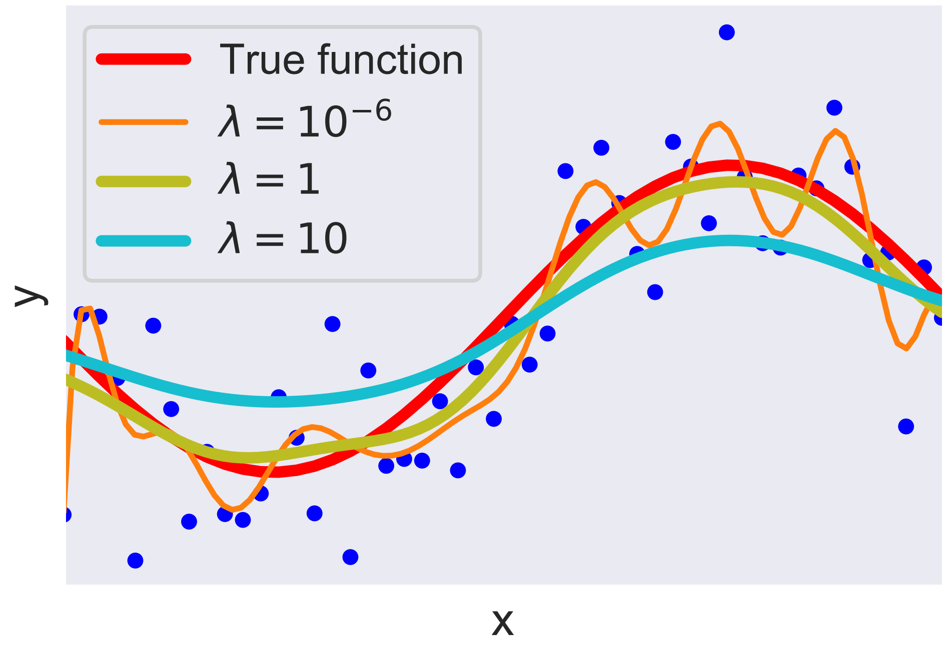
$$\mathbb{E}_{P_0} l(\hat{\theta}, \xi) \leq \frac{1}{N} \sum_{i=1}^{N} l(\hat{\theta}, \xi_i) + \mathcal{O}(\frac{1}{\sqrt{N}})$$



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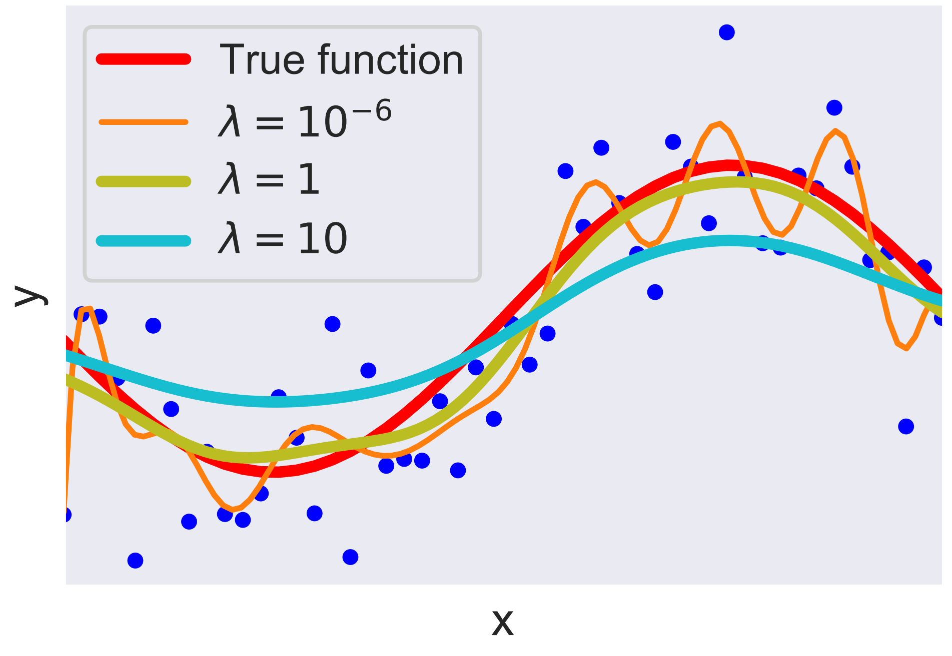

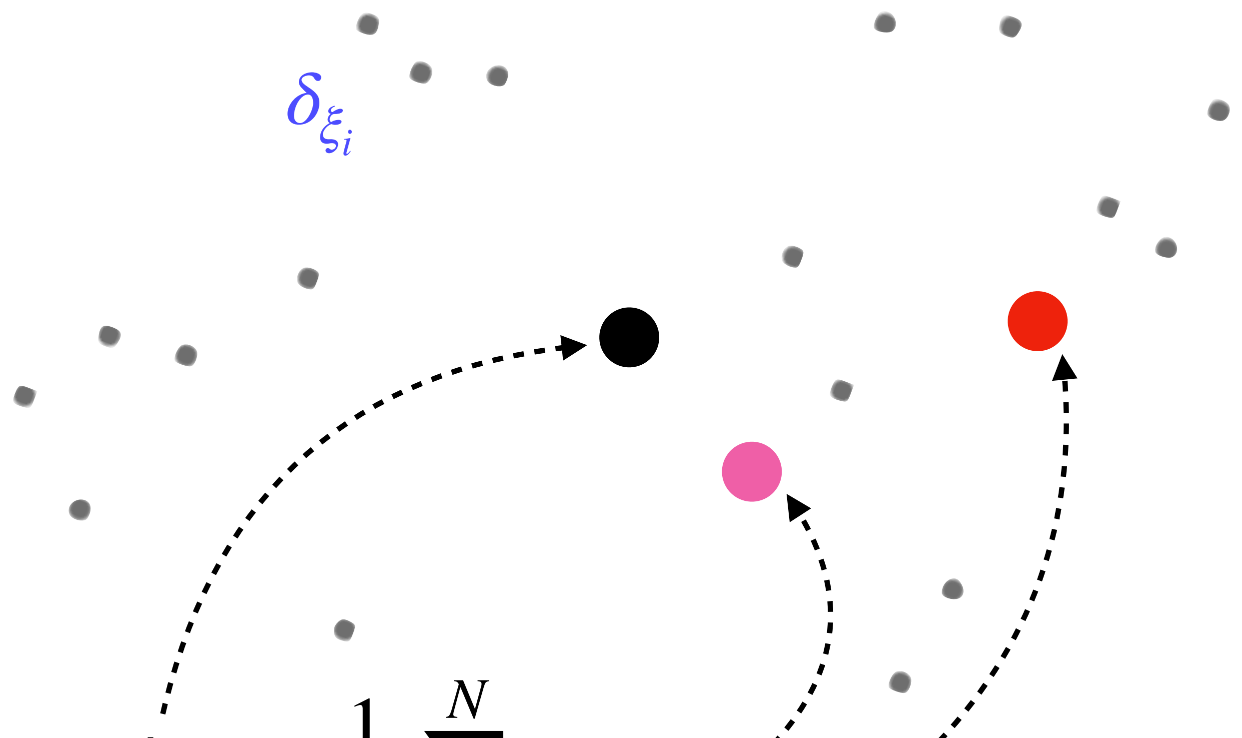

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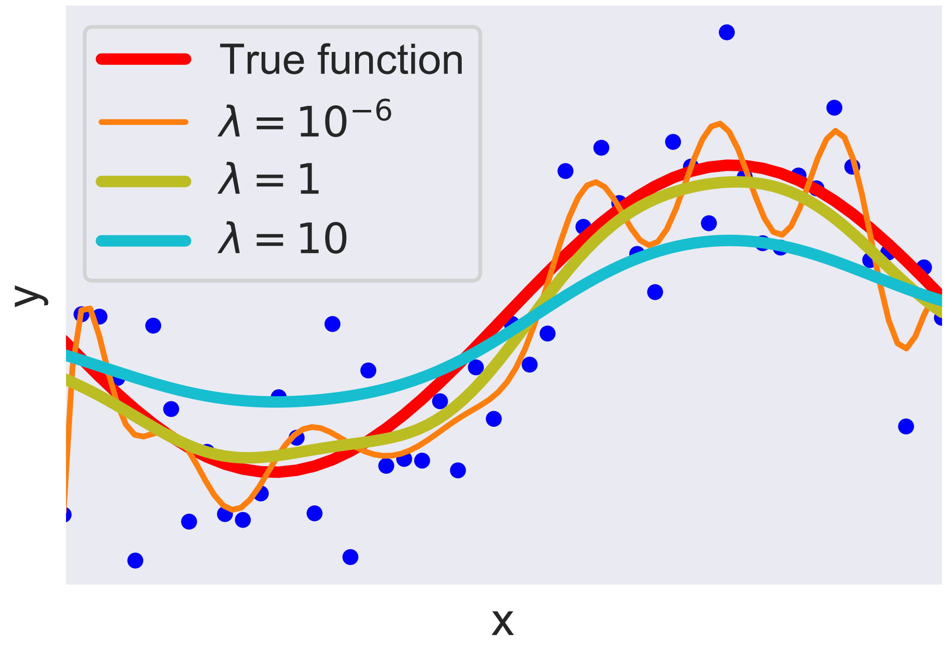

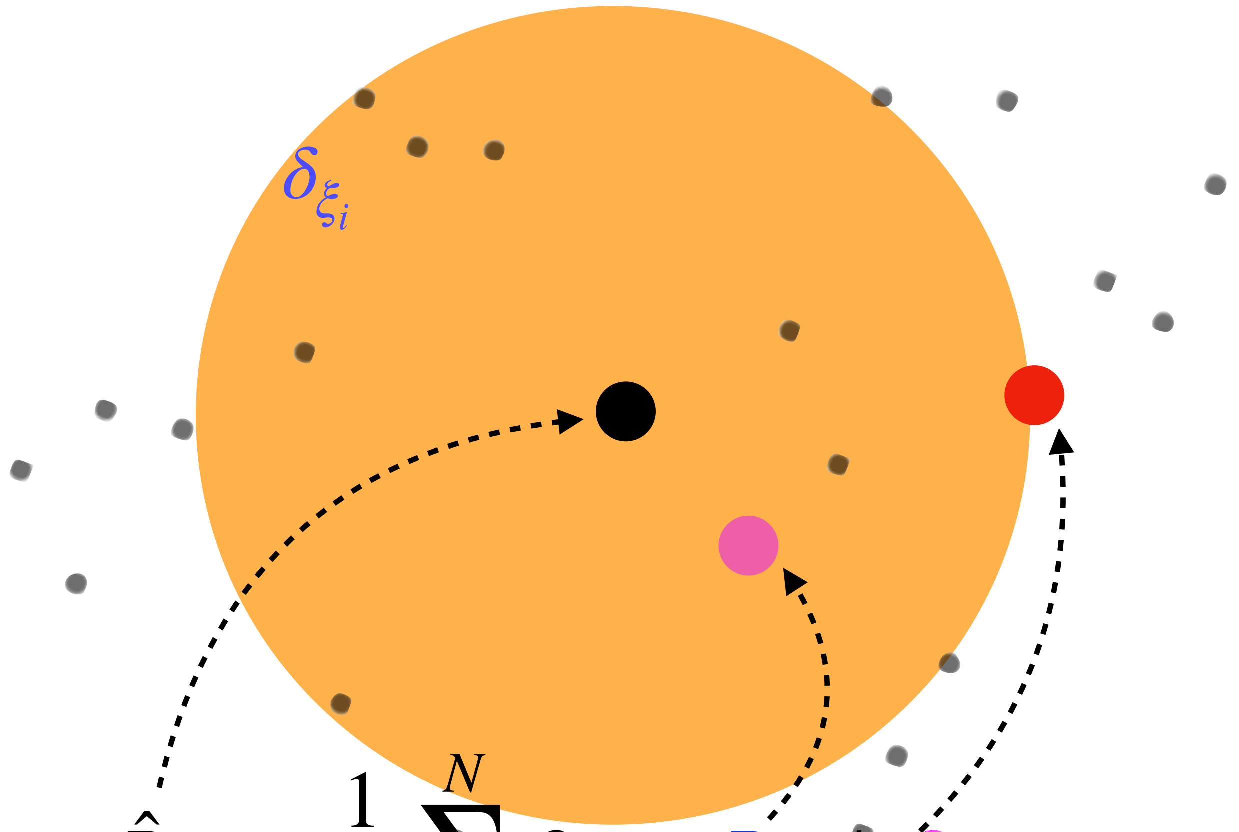

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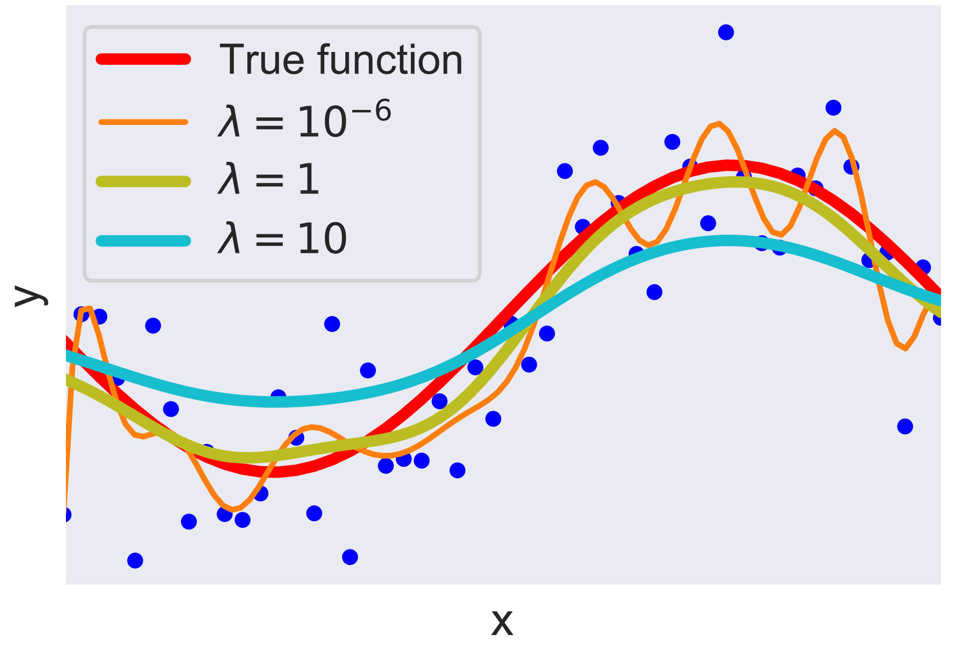

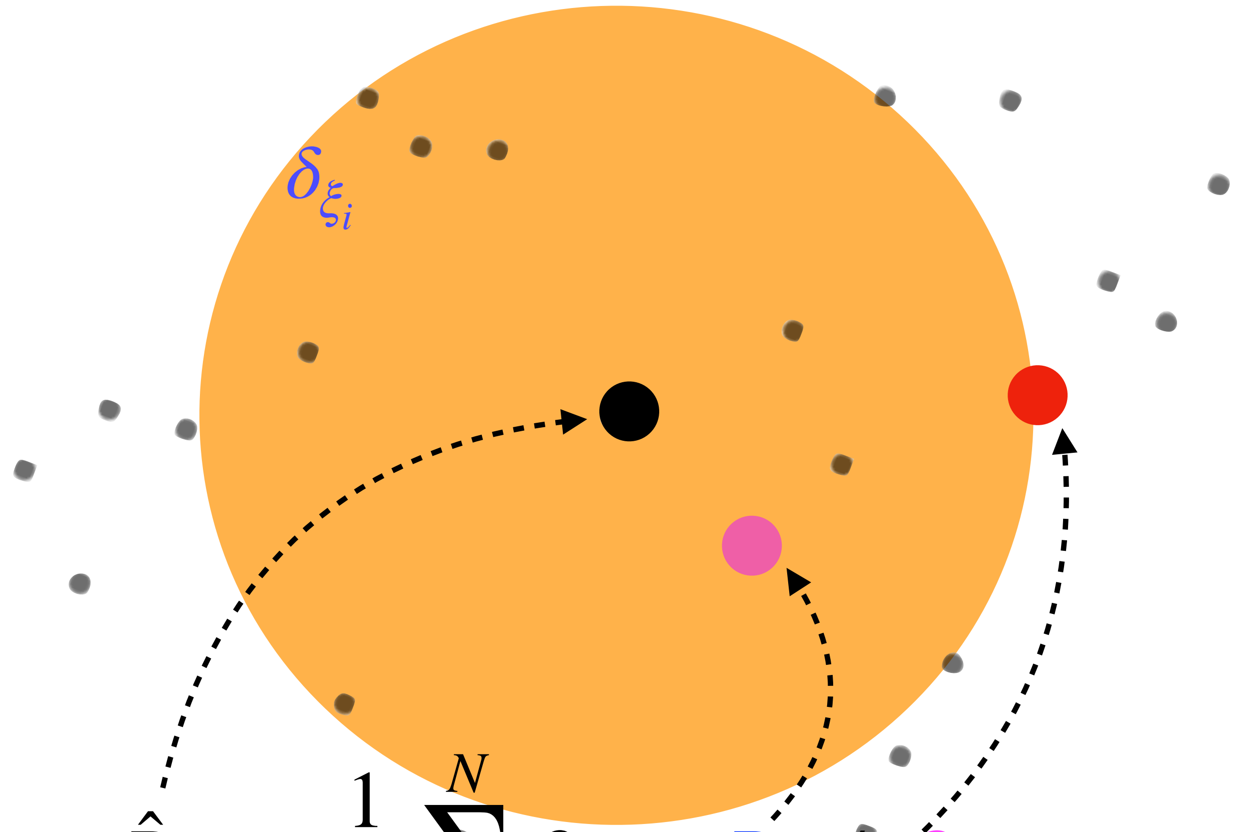

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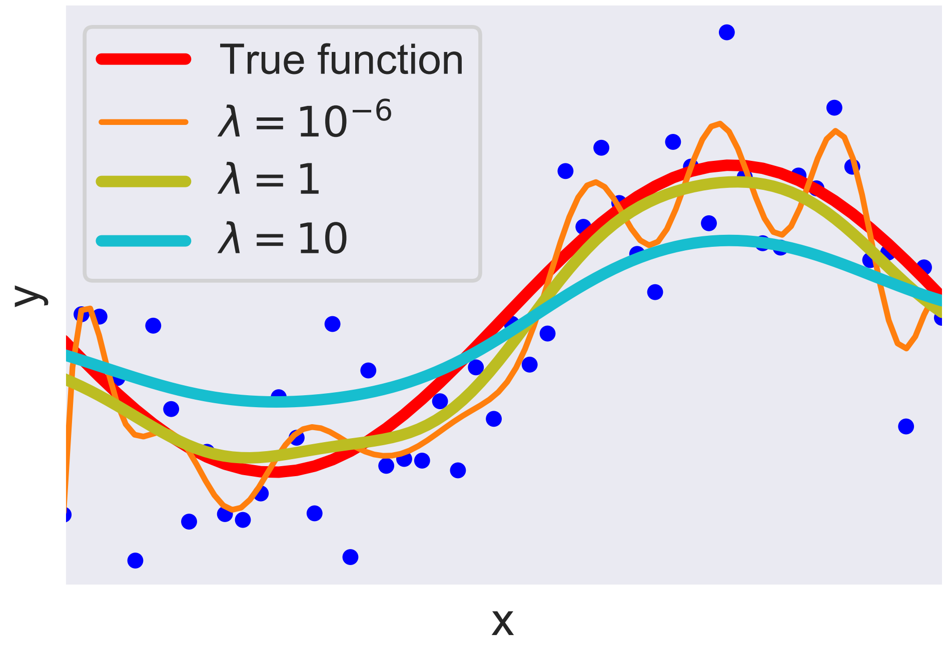

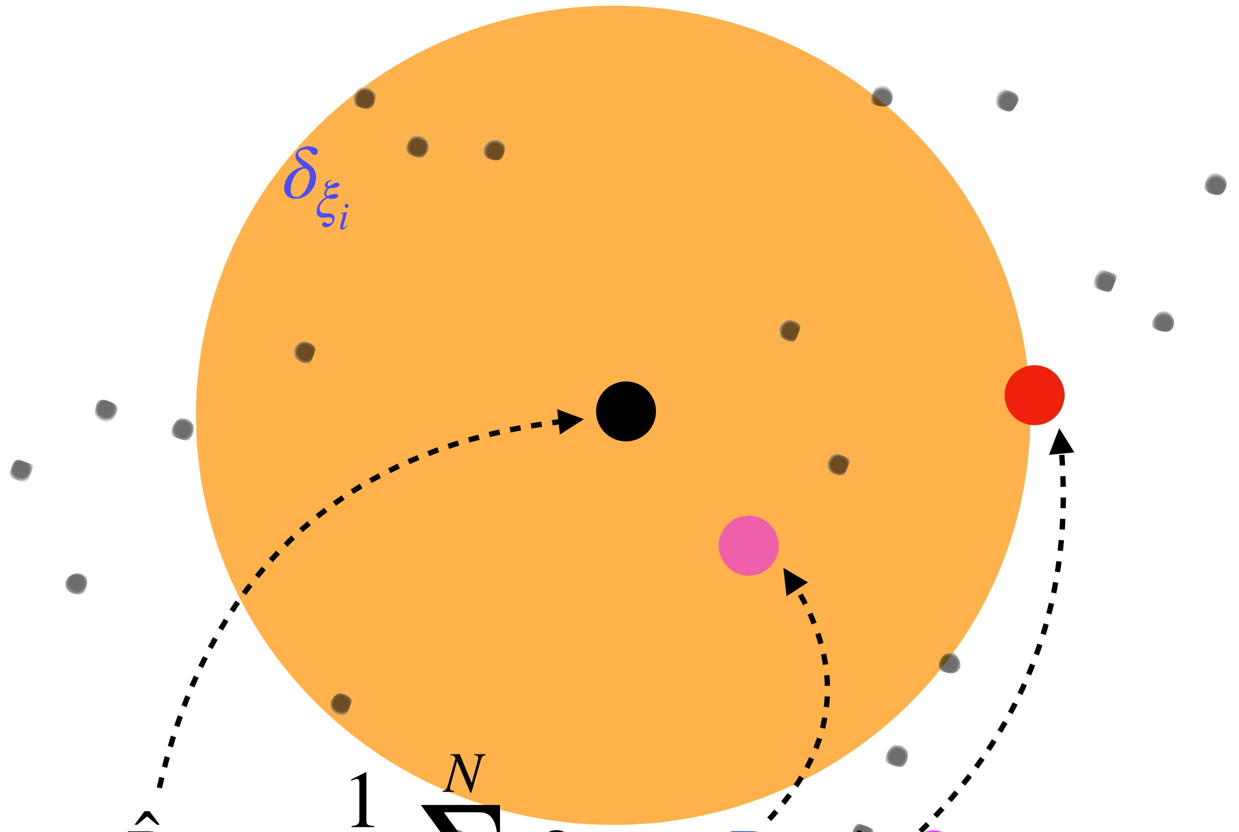

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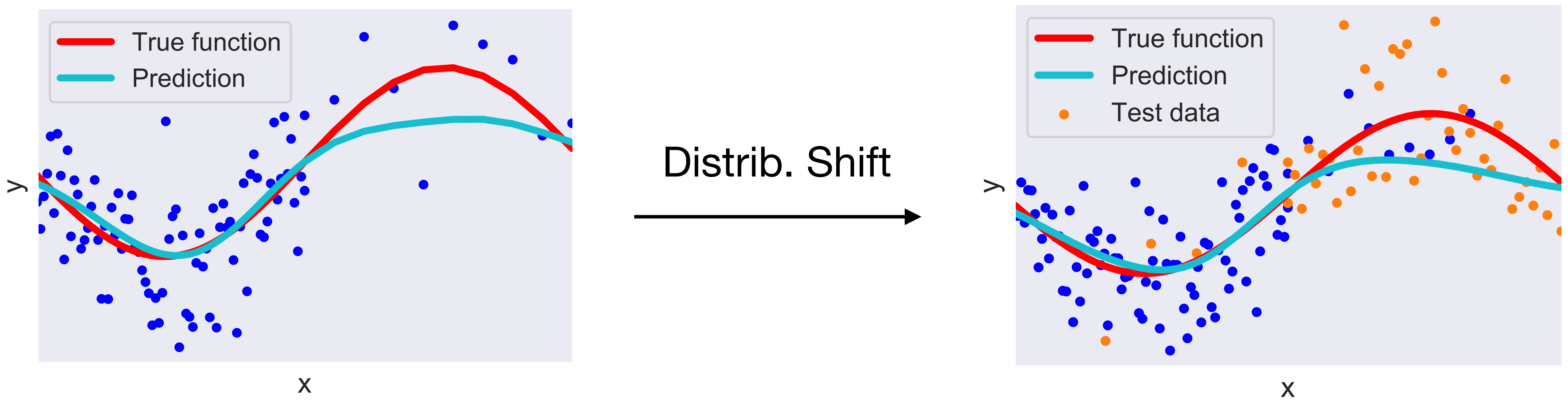

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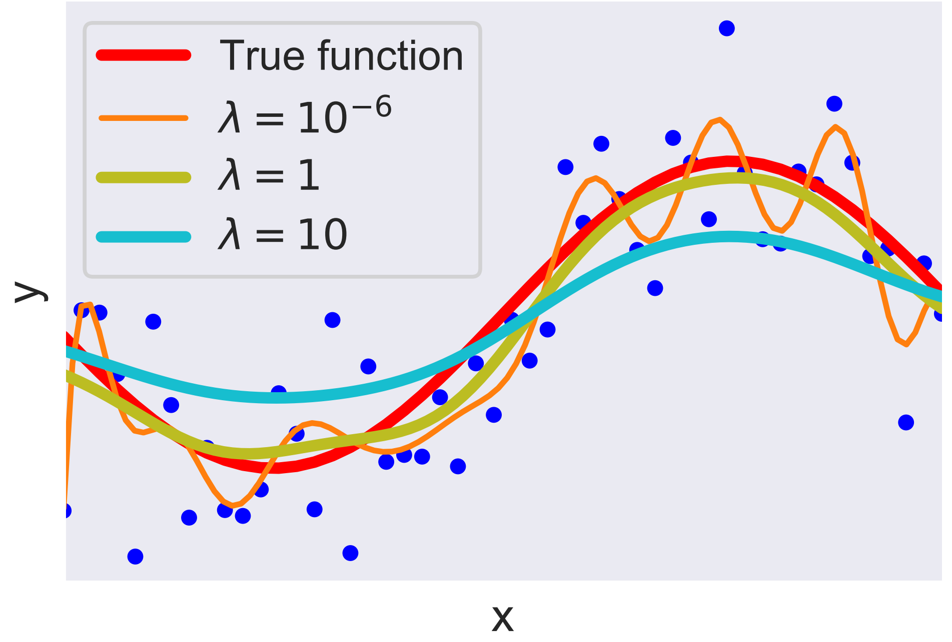

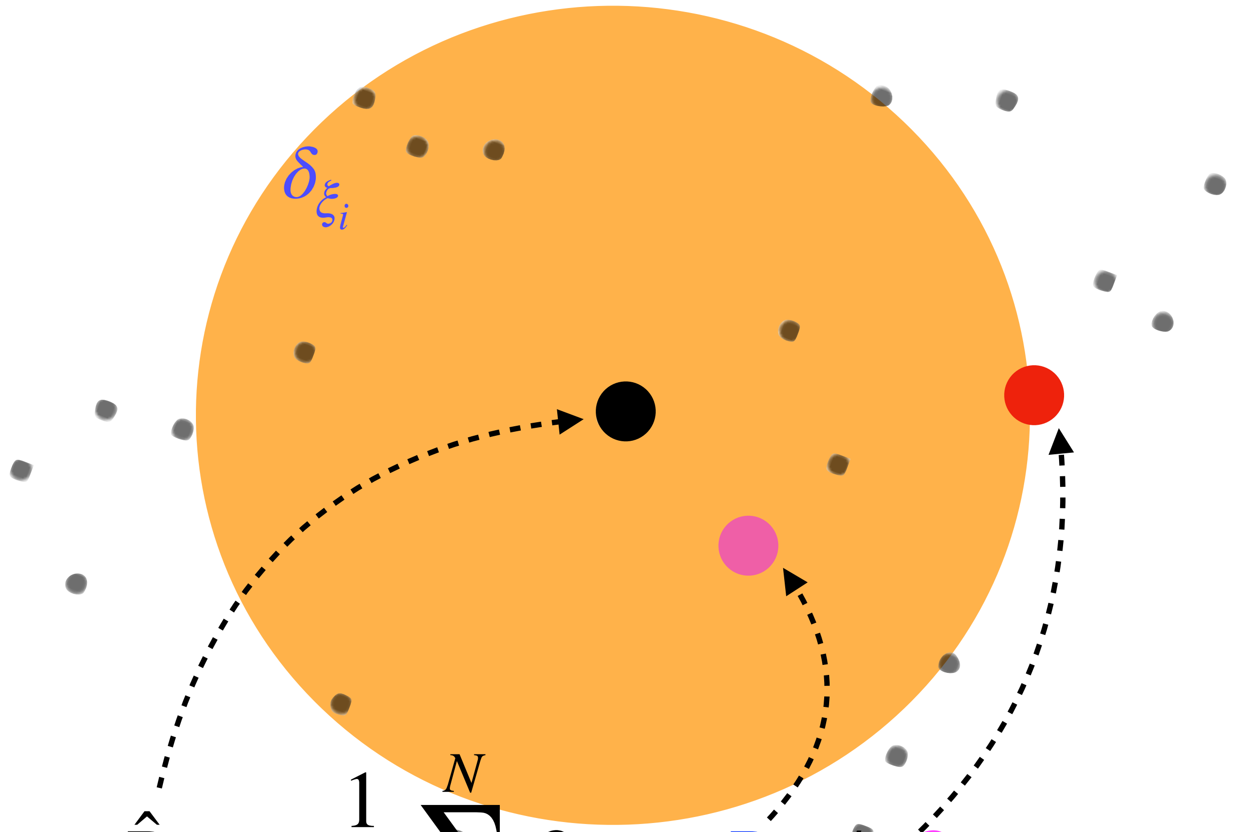

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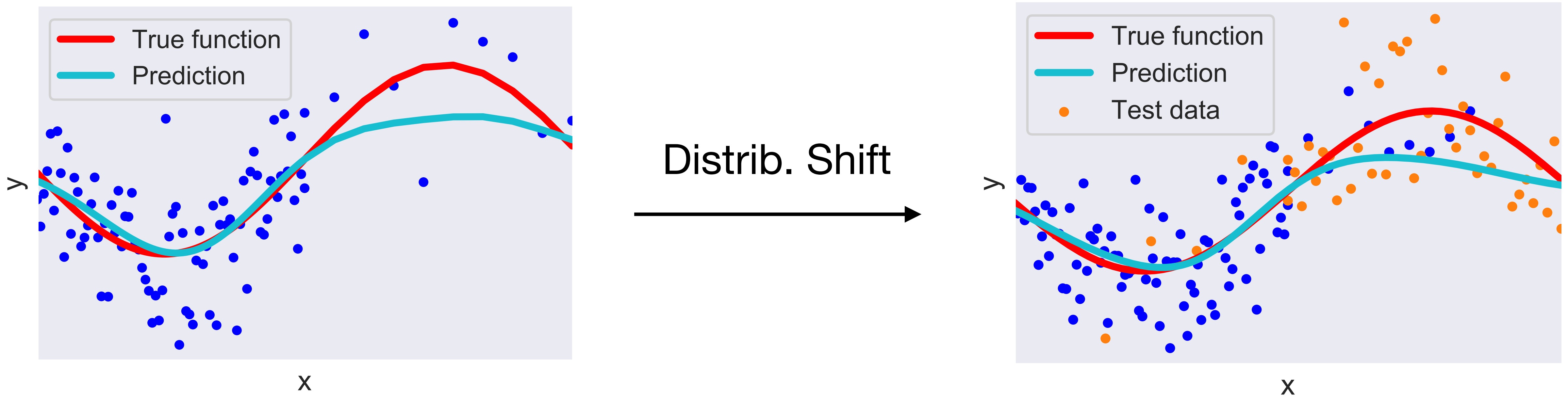

Why study new geometry?

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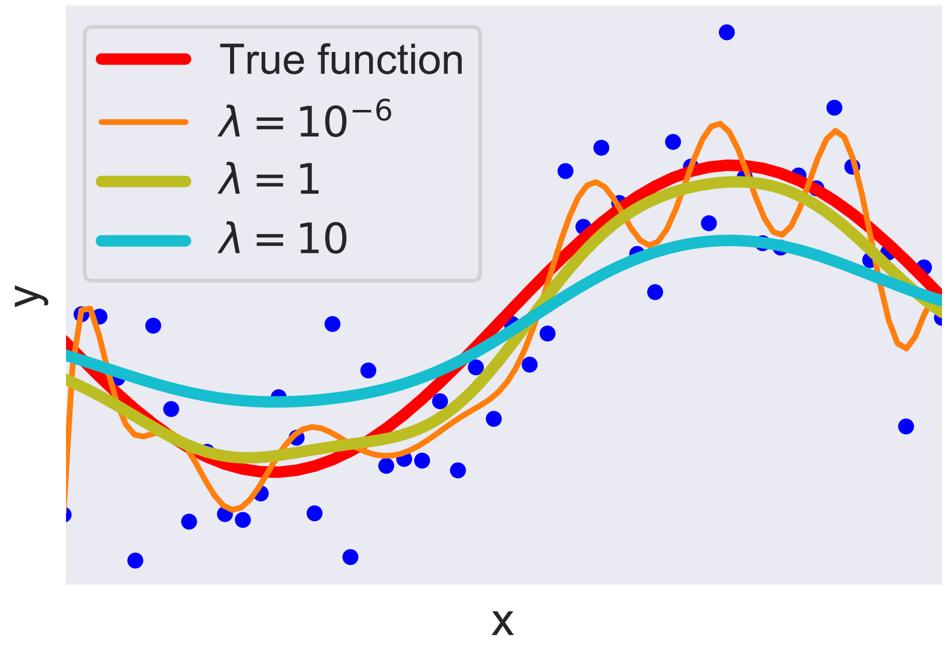

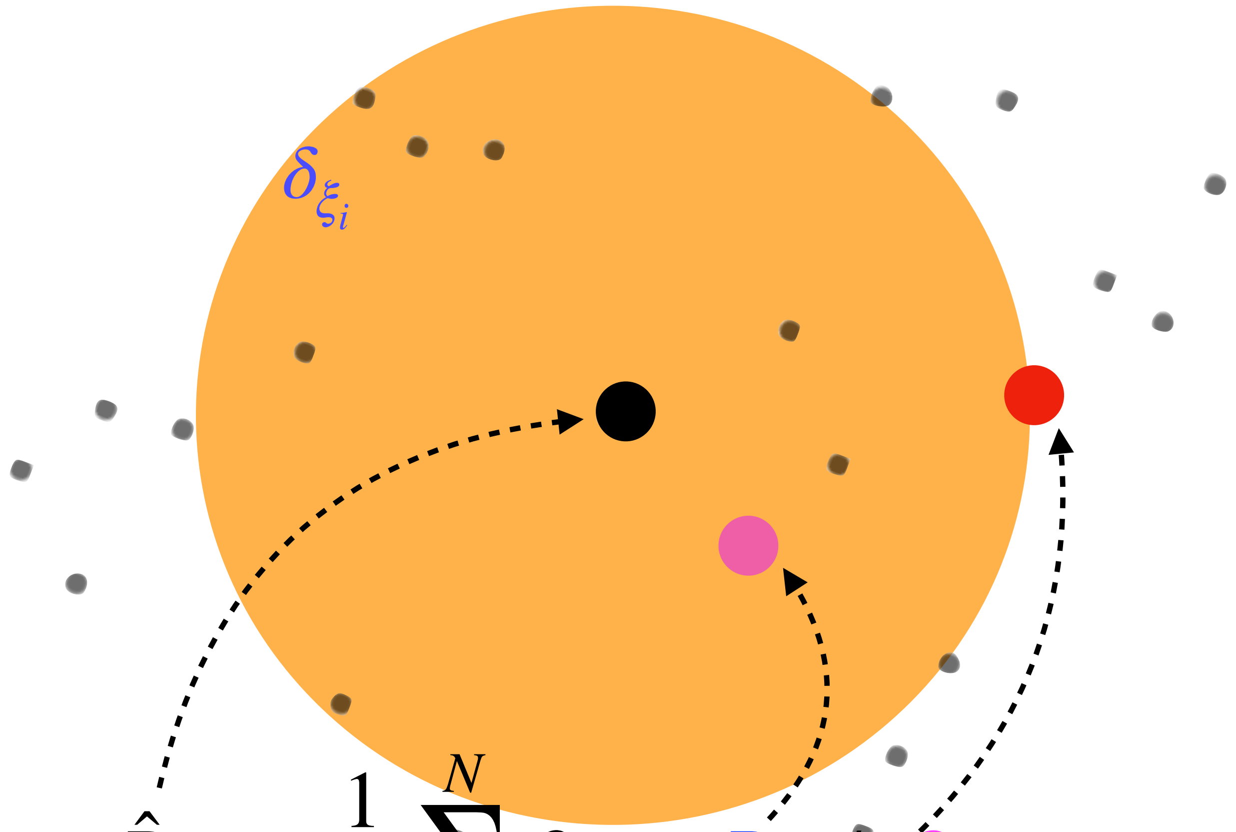

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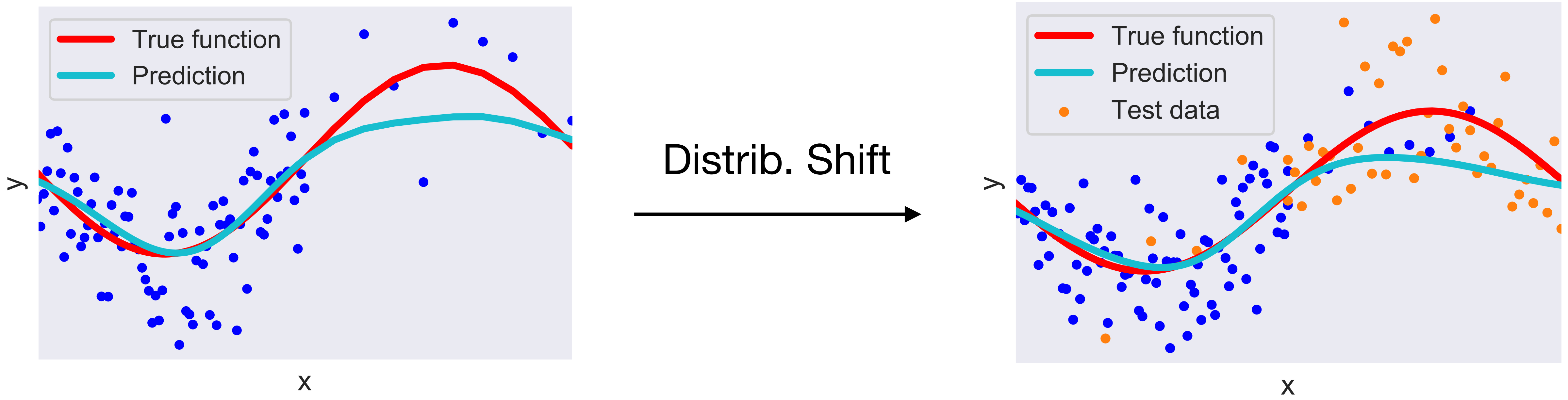

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New geometries leading to new fields of research and breakthroughs:

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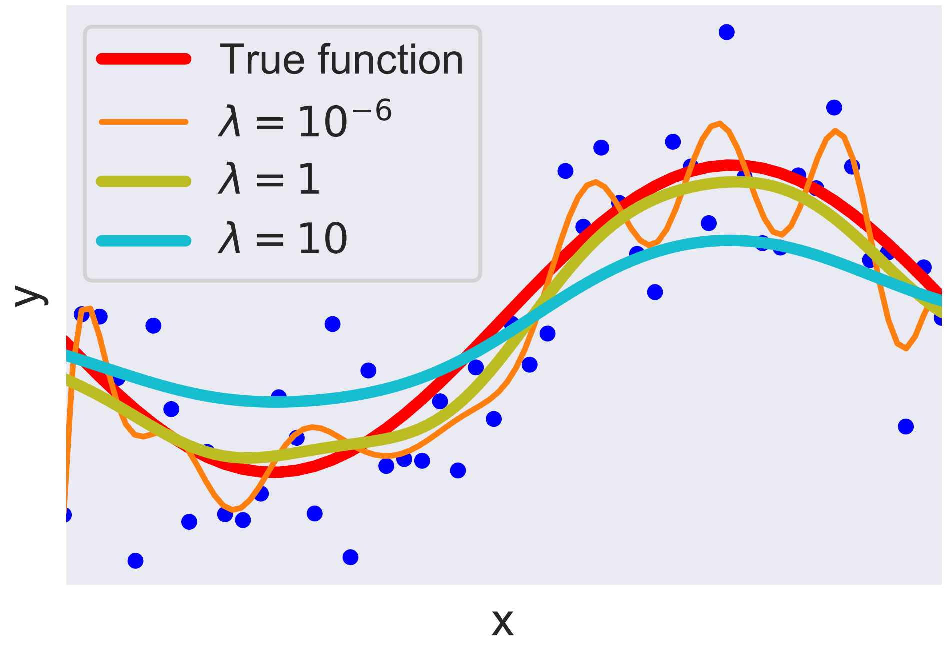

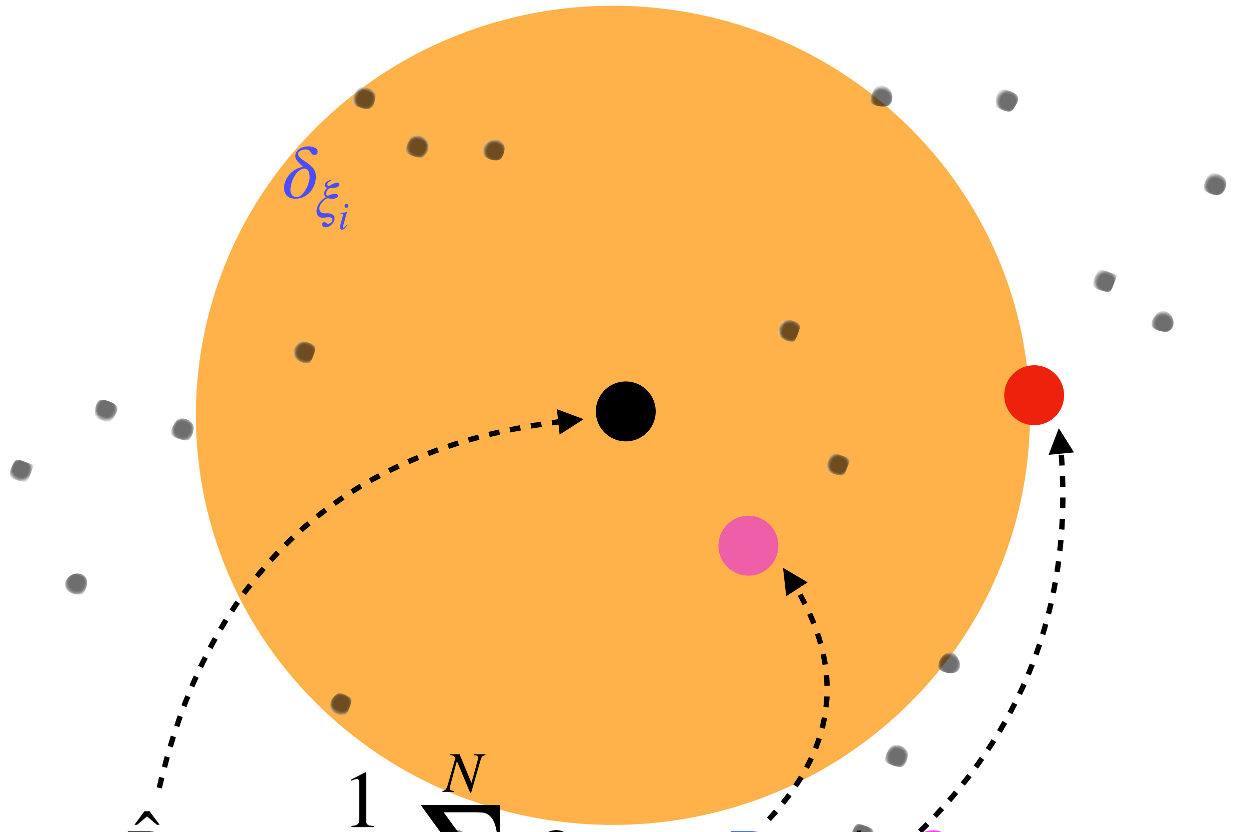

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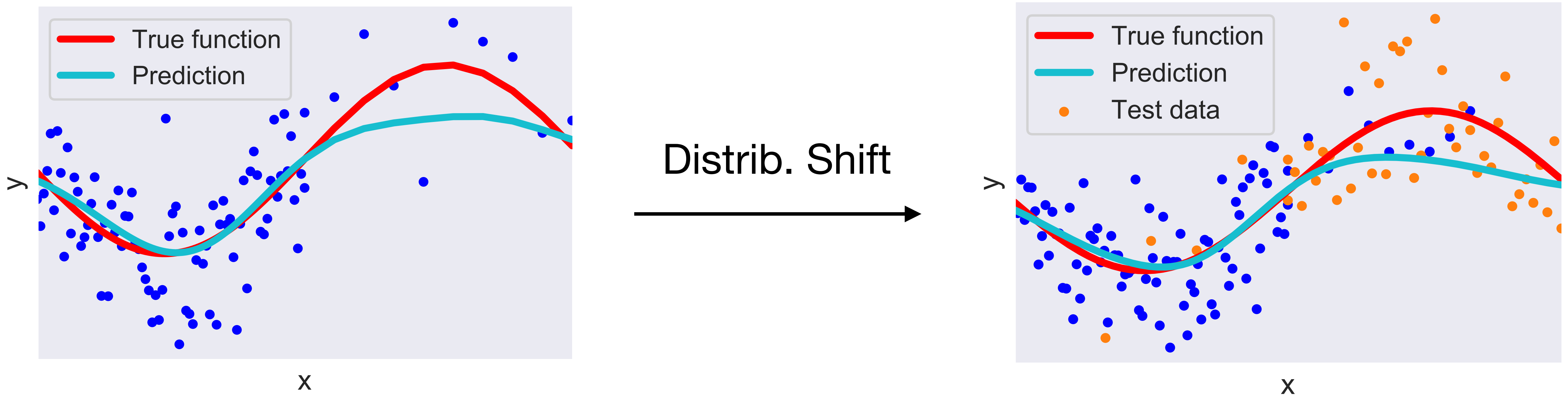

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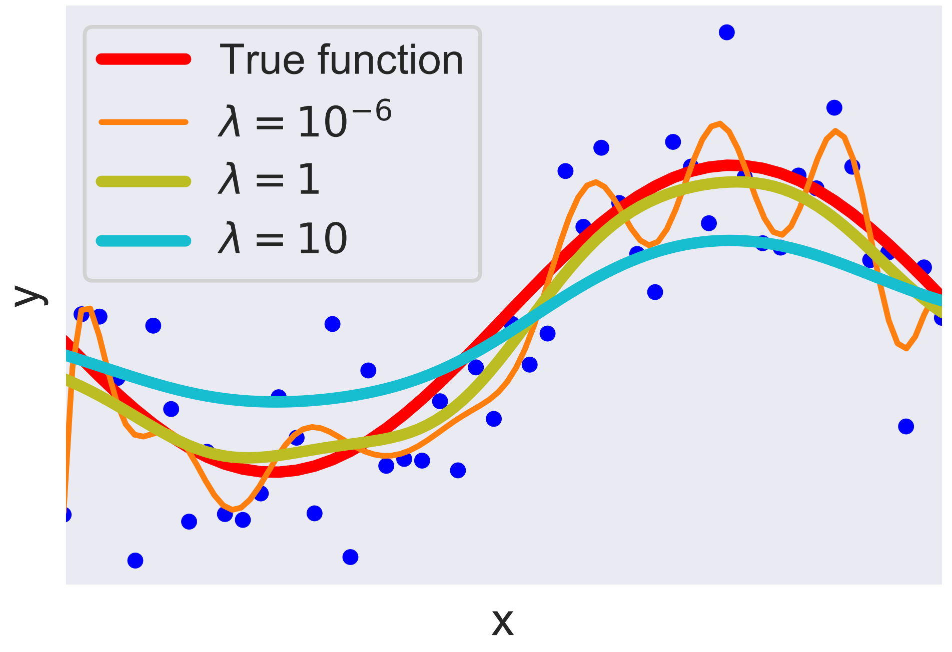

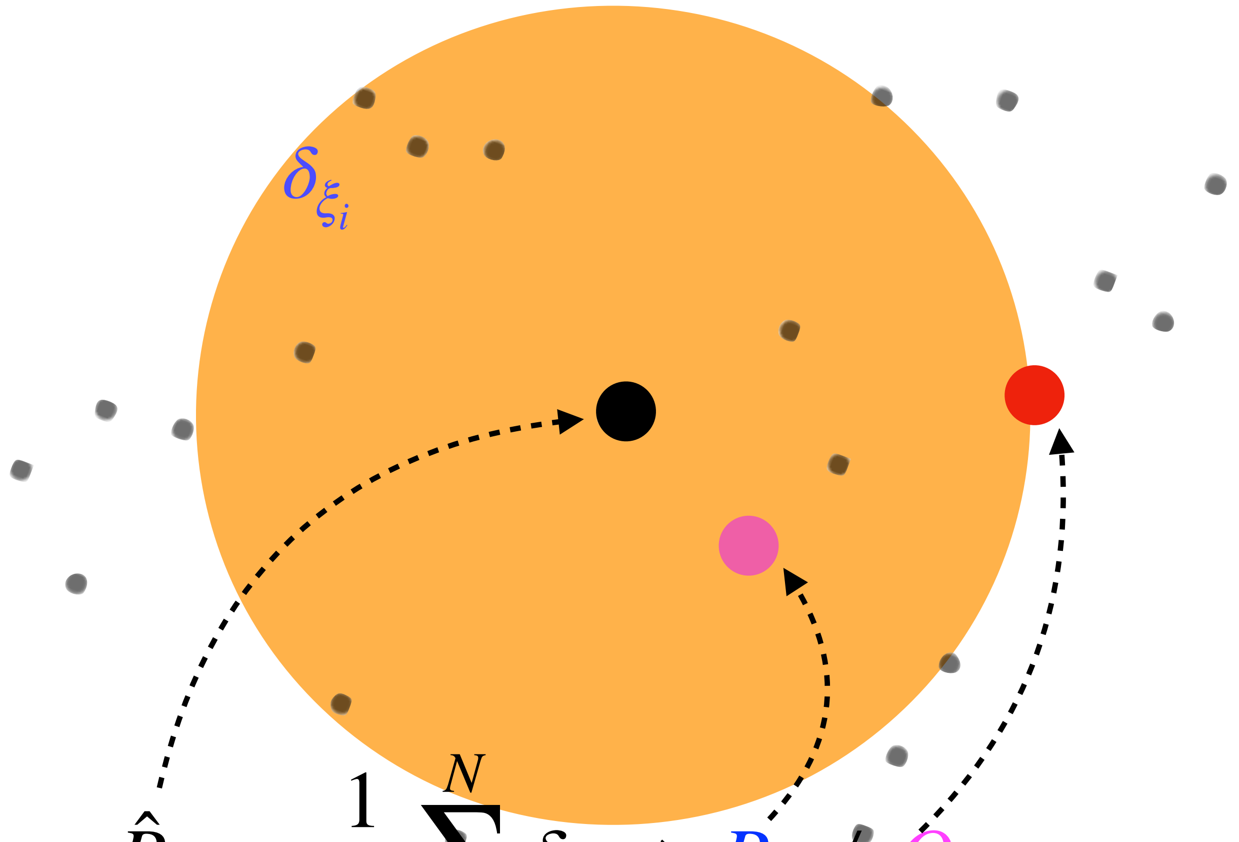

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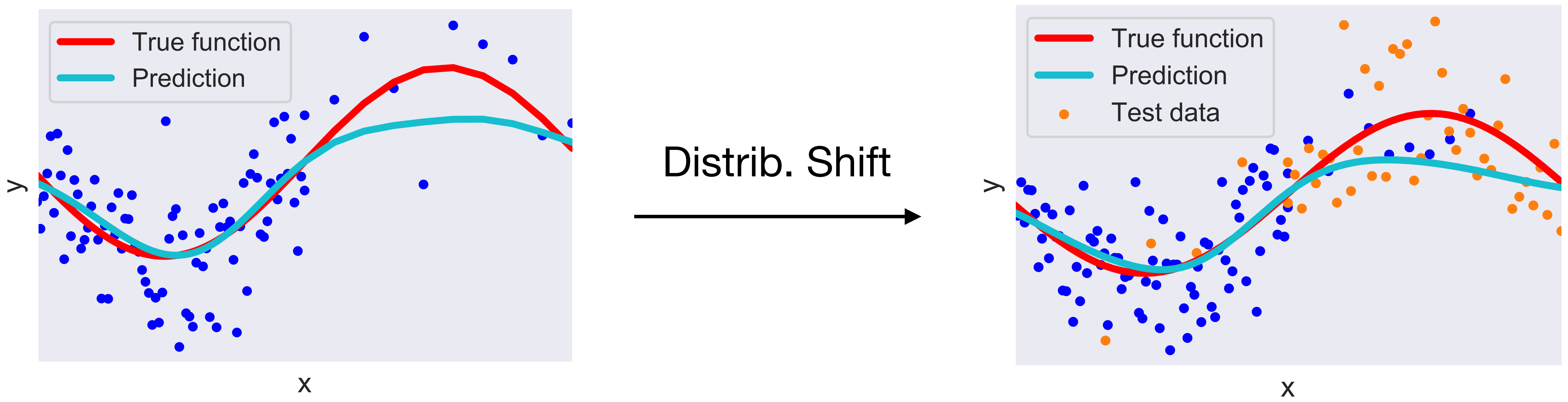

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Wasserstein Gradient flow [F. Otto et al.] e.g. Fokker-Planck equation as Wasserstein flow

Figure credit: H. Kremer

Background: Wasserstein Geometry

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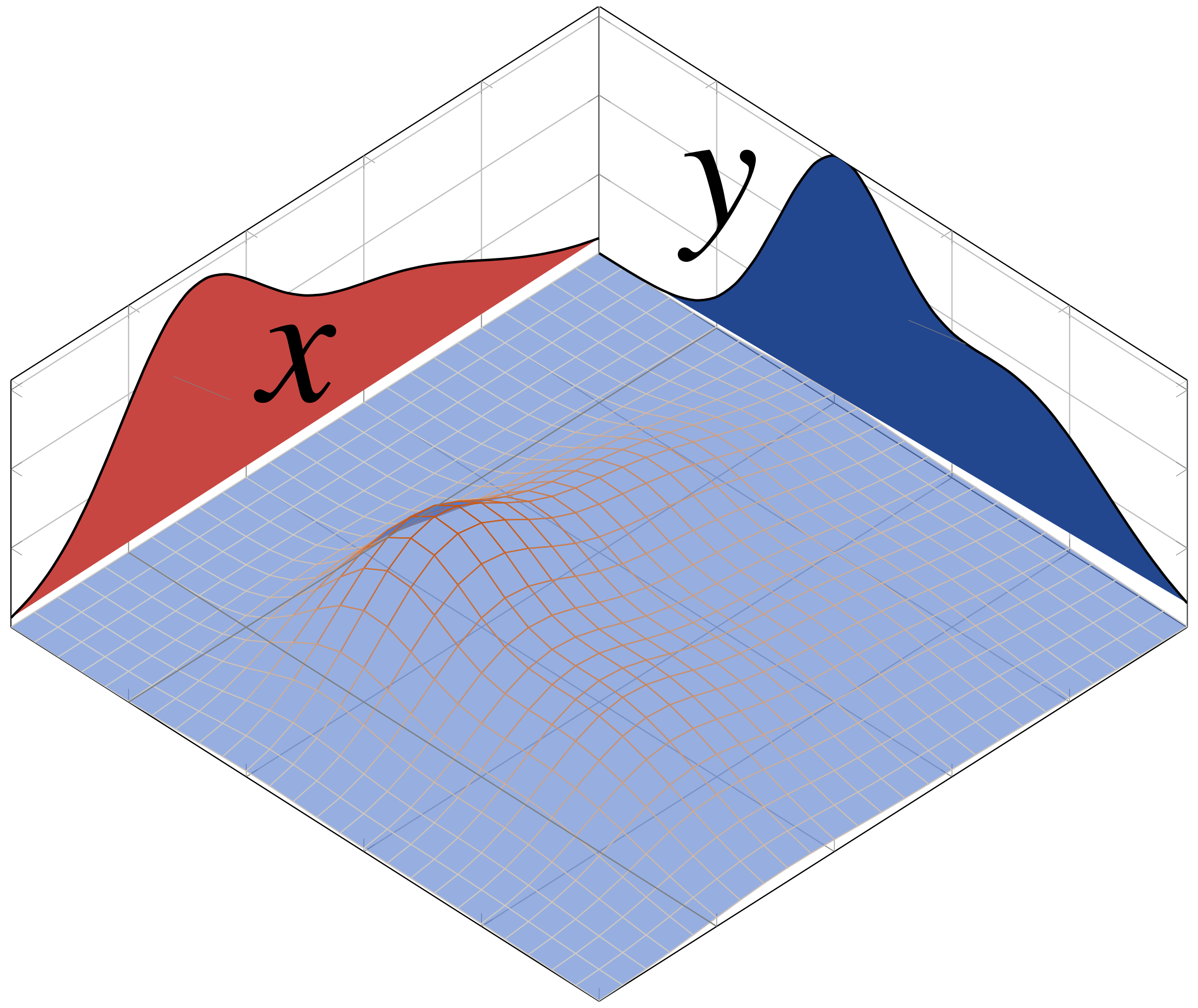
Definition. The p-**Wasserstein distance** between probability measures P, Q on $\mathbb{R}^d$ (with p finite moments, $p \geq 1$) is defined through the following Kantorovich problem



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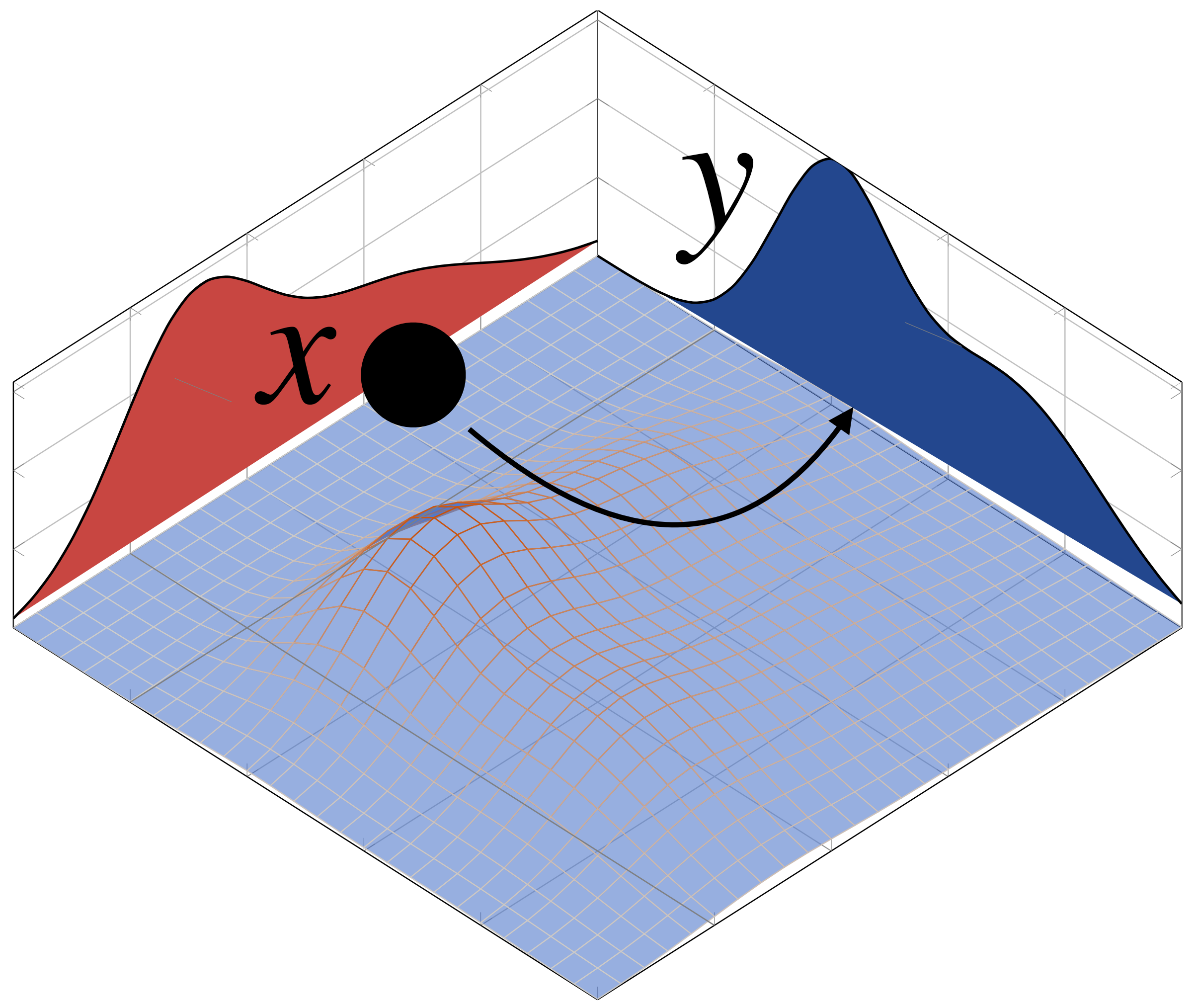

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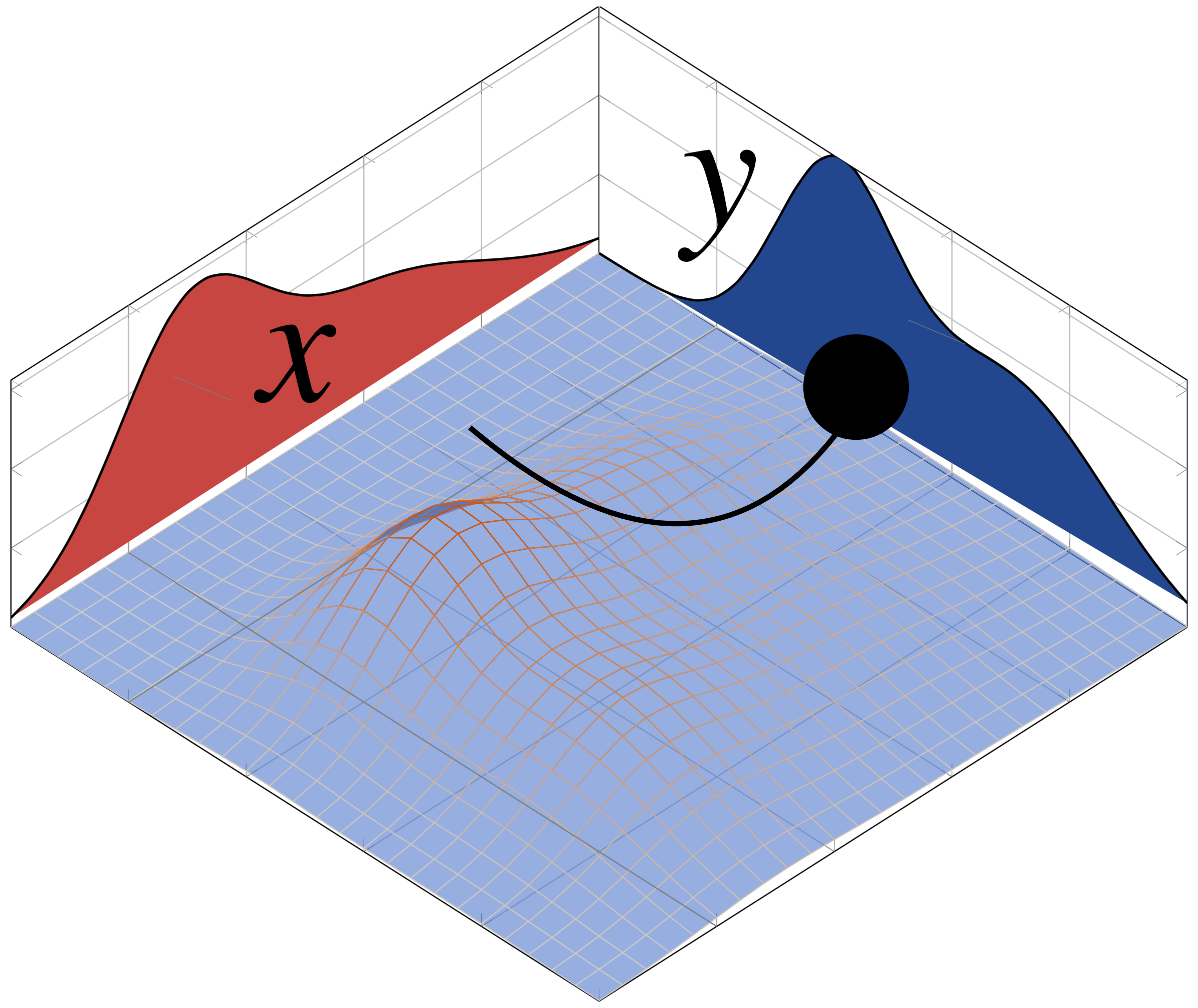

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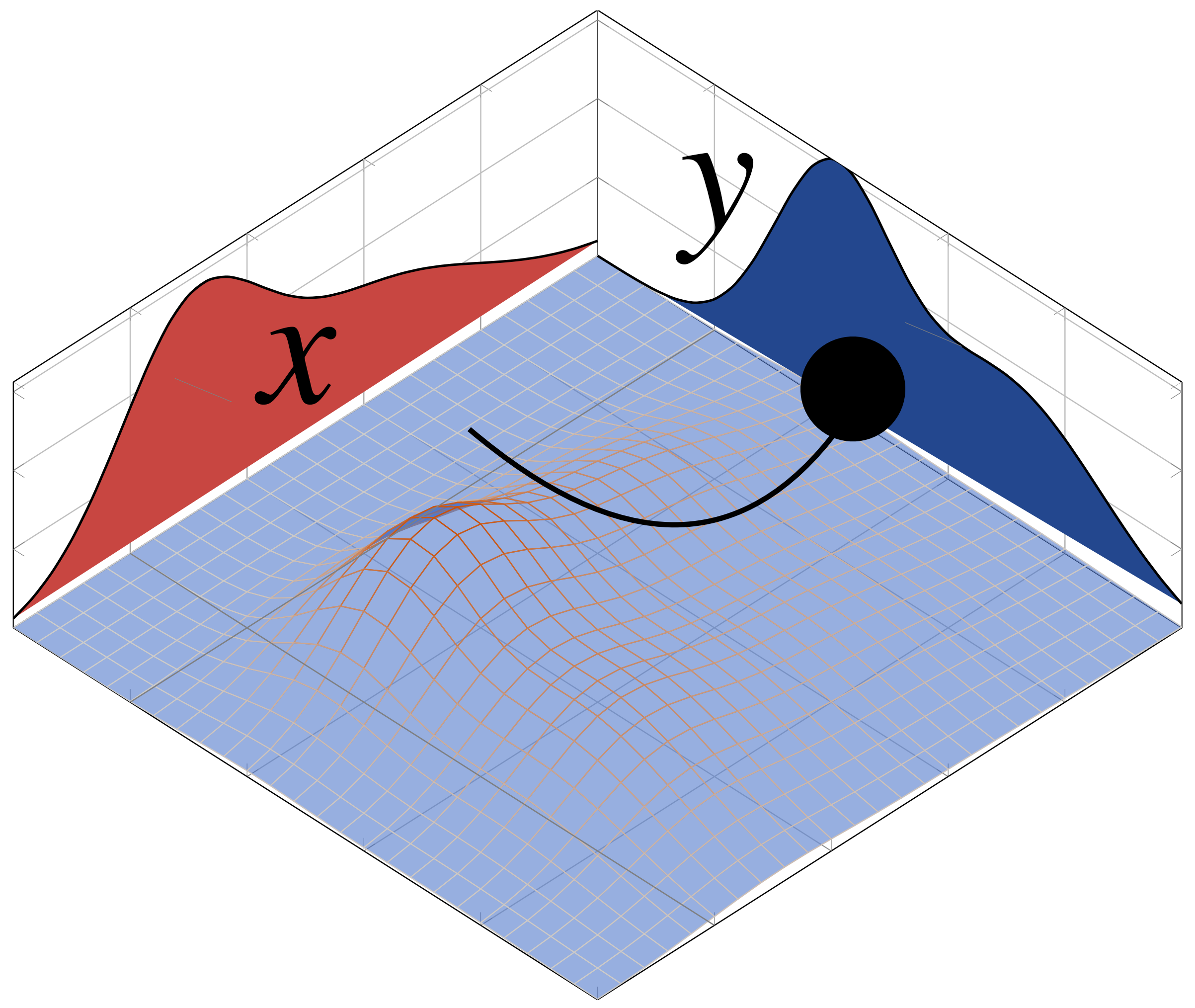

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(**Dual Kantorovich problem**)

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

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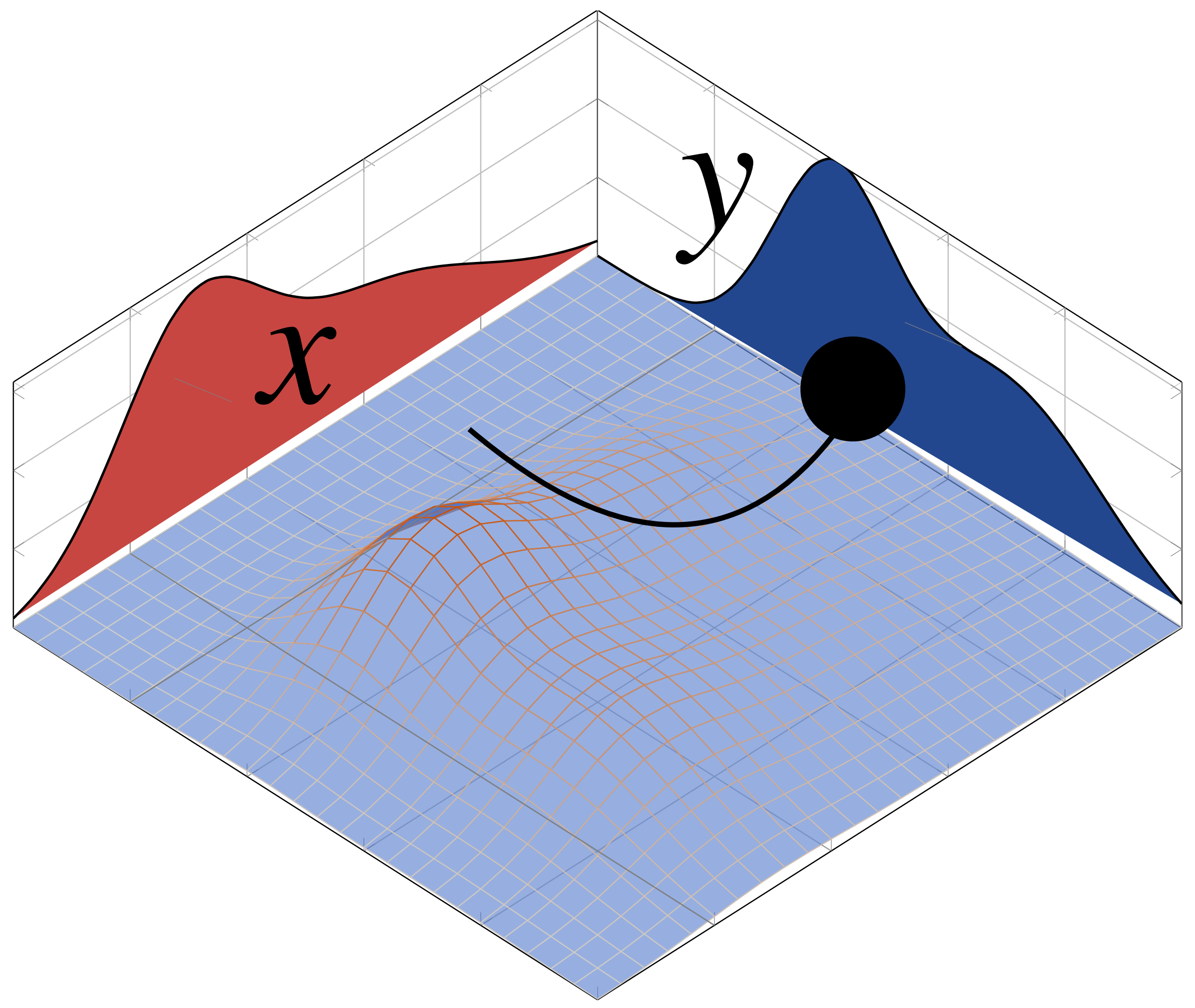

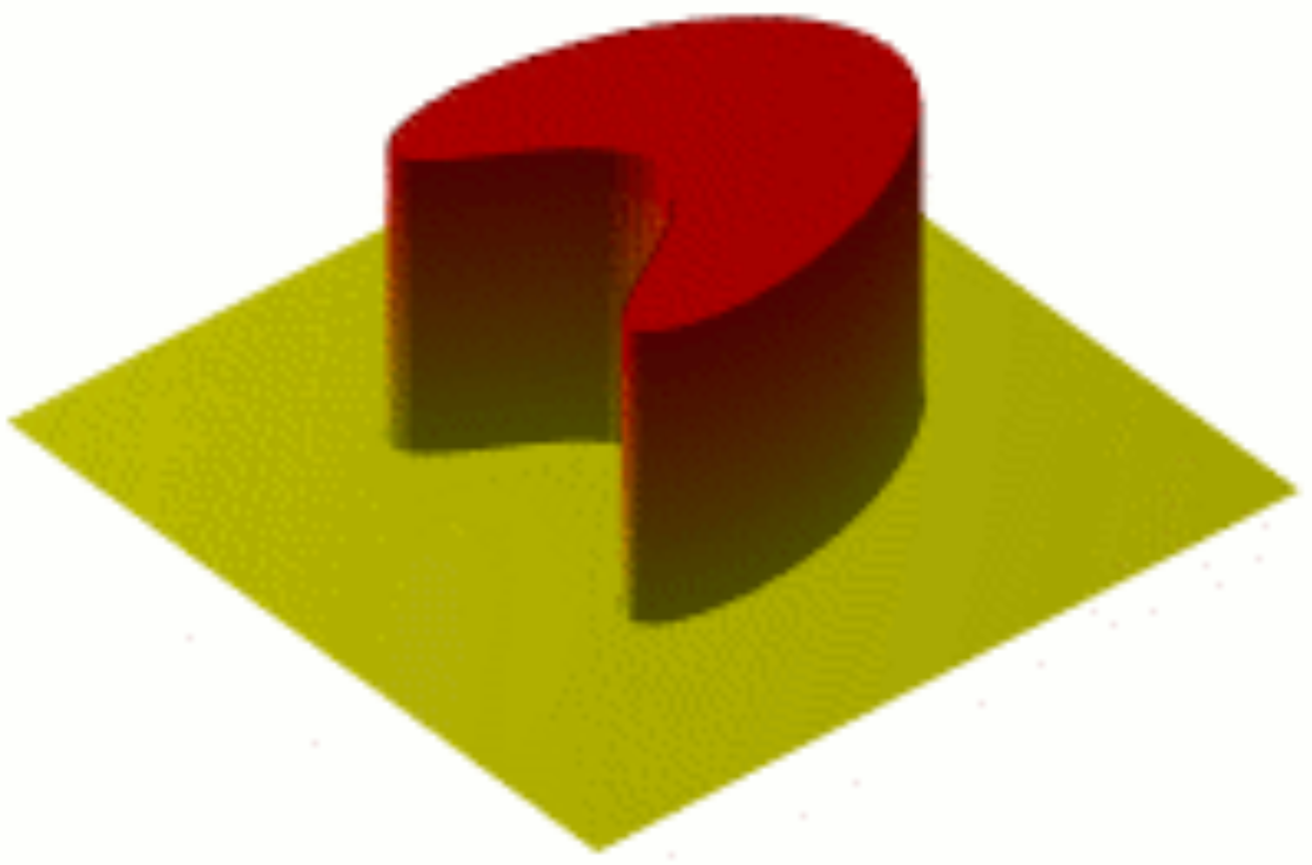

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Dynamic formulation: *Benamou–Brenier*

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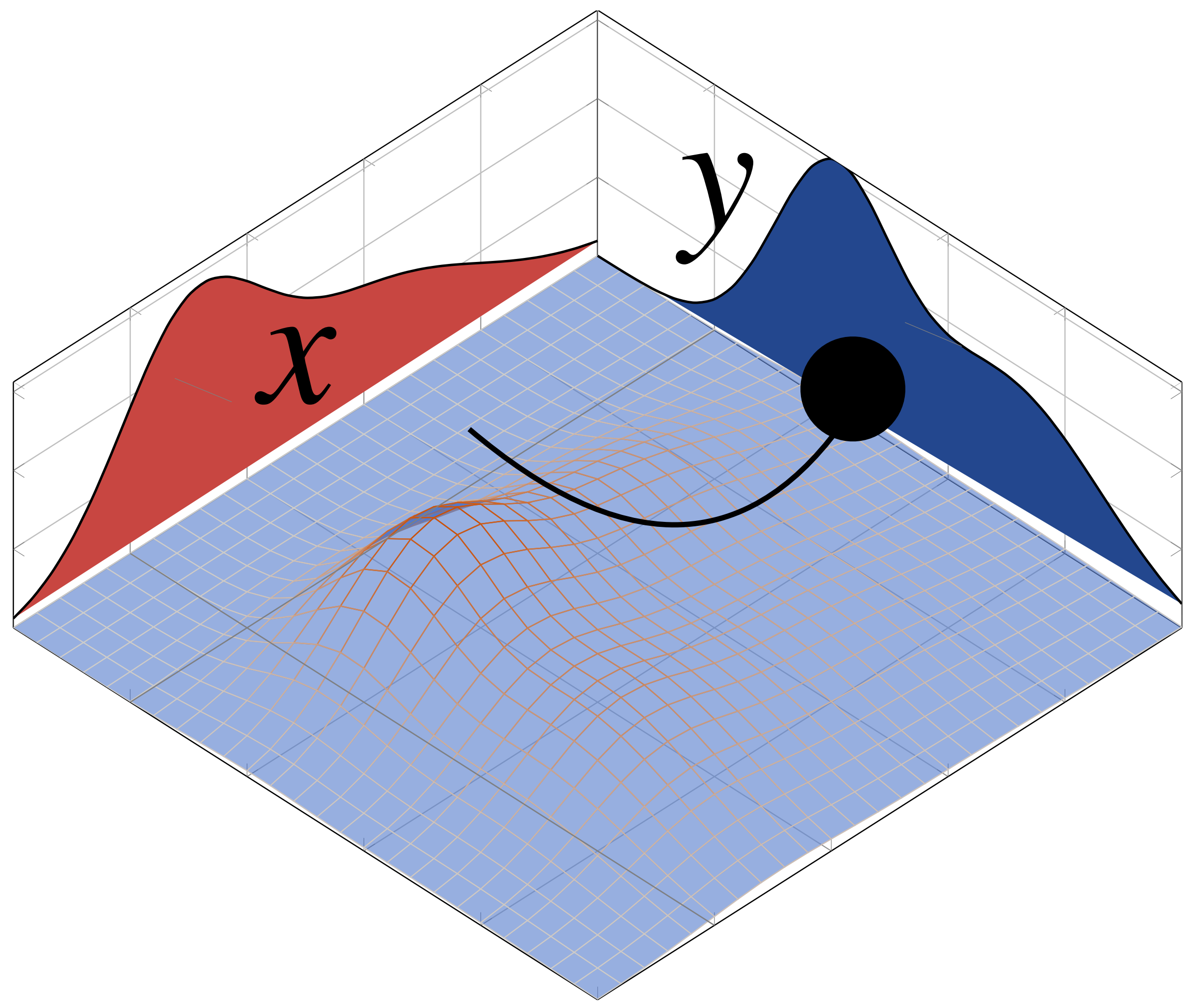
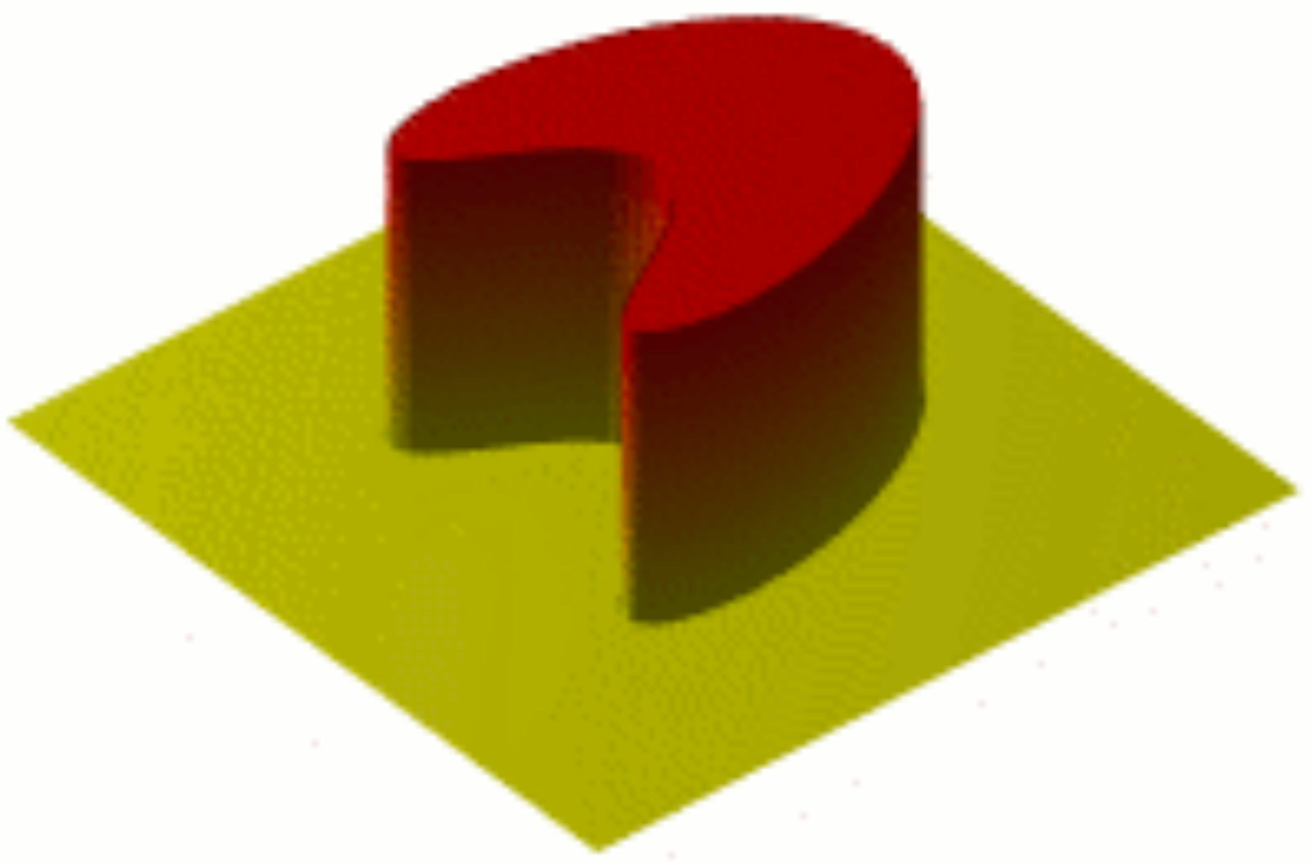
Example. Entropy-OT [Cuturi 2013] Duality leads to faster computation

$$\inf \int c d\Pi + \lambda D_\phi(\Pi || P \otimes Q)$$





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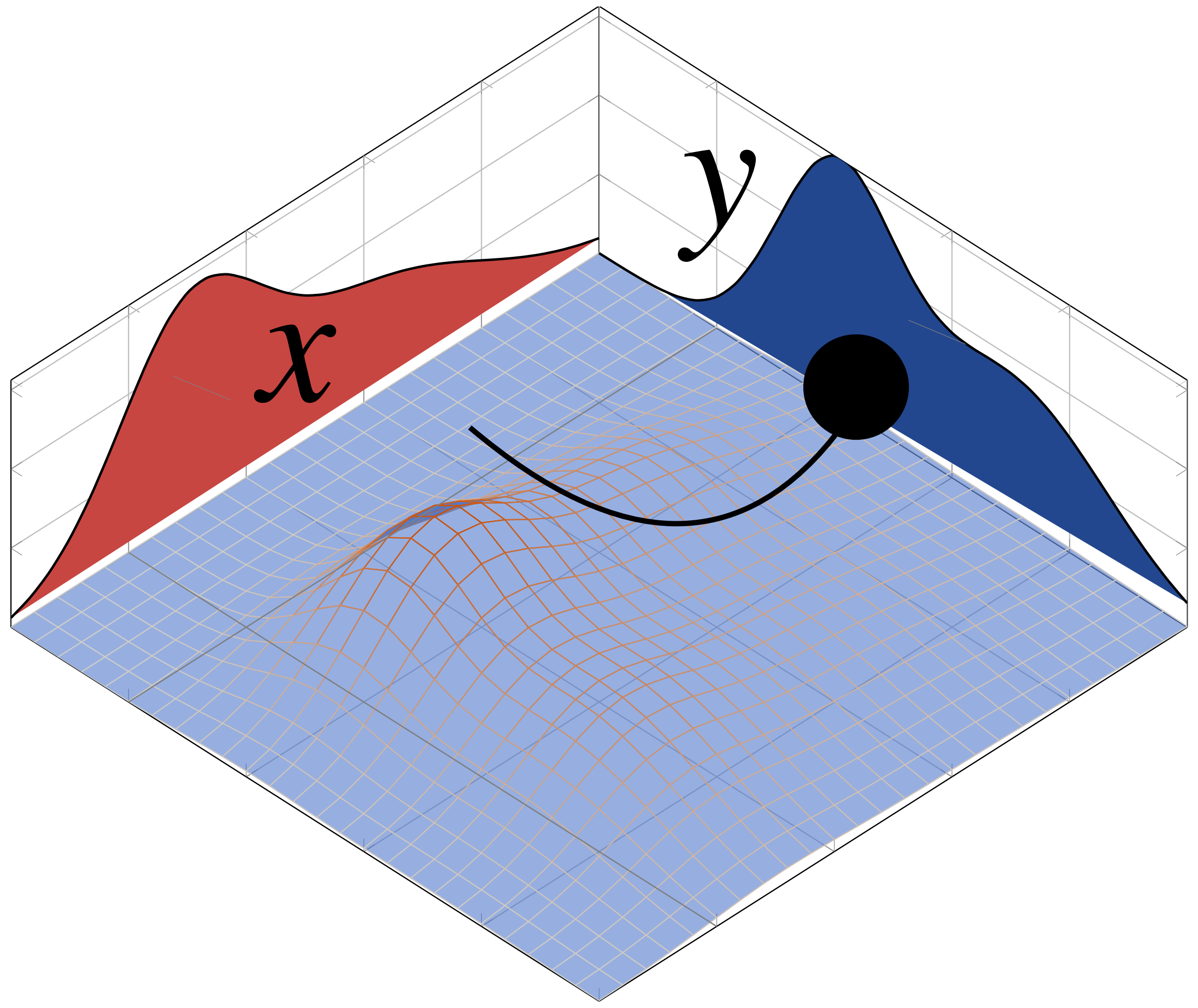
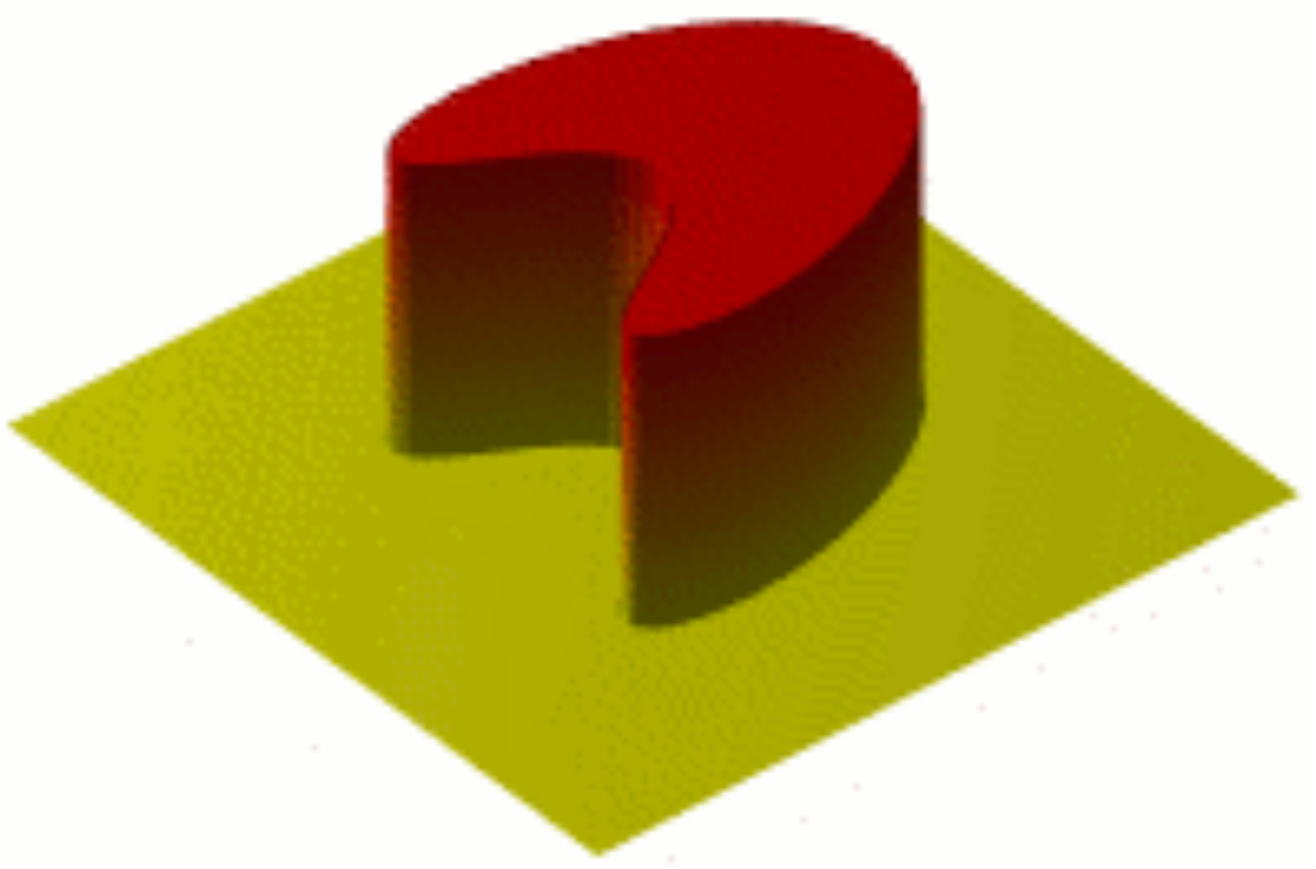
Dynamic formulation: *Benamou–Brenier*

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

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

$$\inf \int c\,d\Pi + \lambda D_\phi(\Pi || P \otimes Q)$$





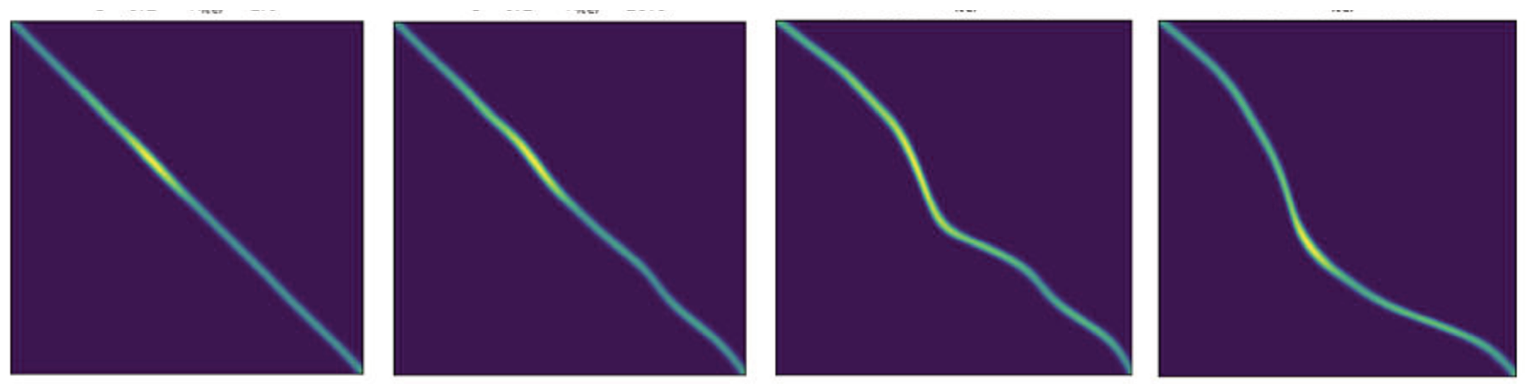


Figure credit: Wiki., M. Cuturi, A. Genevay

Background: “Kernel Geometry”

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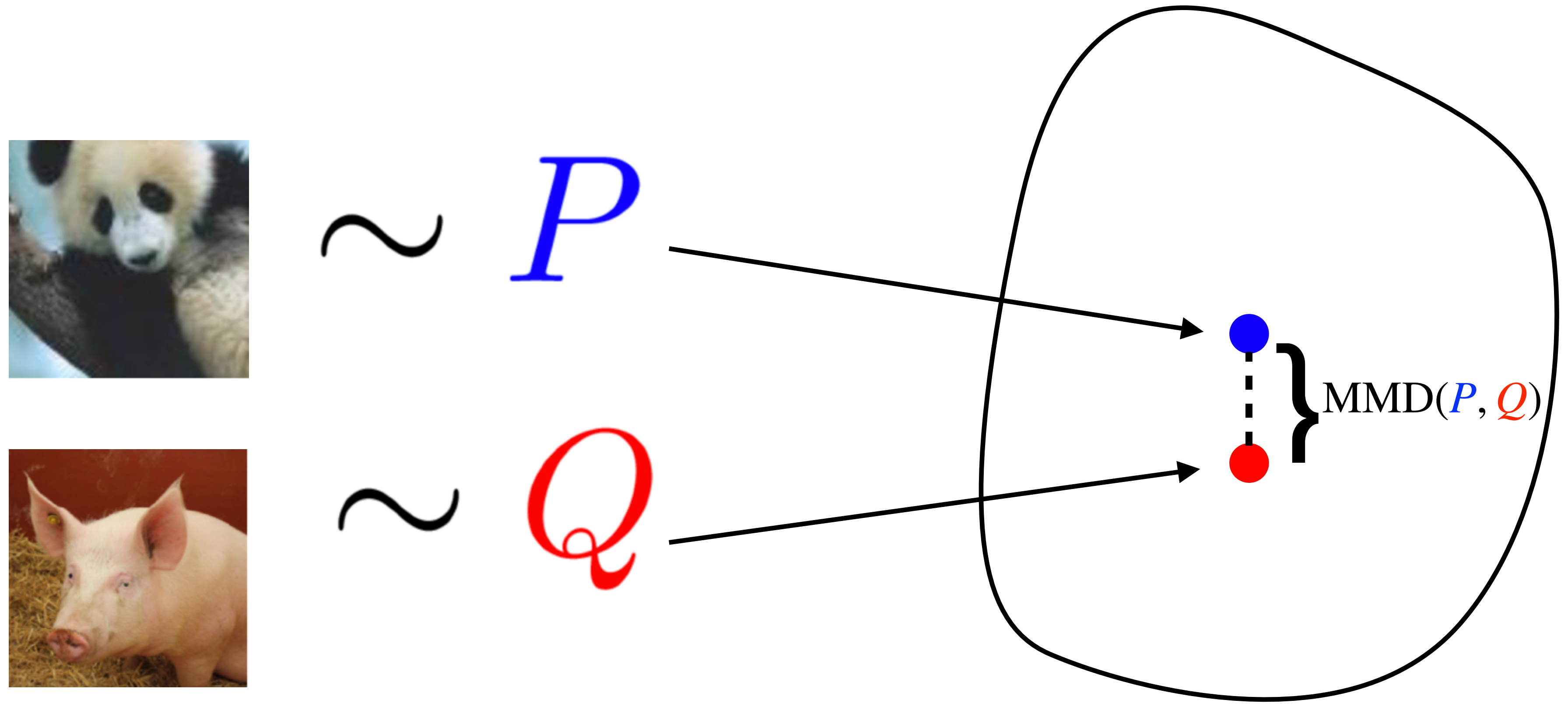
Definition. Kernel **Maximum-Mean Discrepancy** (MMD) associated with (PSD) kernel k (e.g., $k(x, x') := e^{-|x-x'|^2/\sigma}$)

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

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



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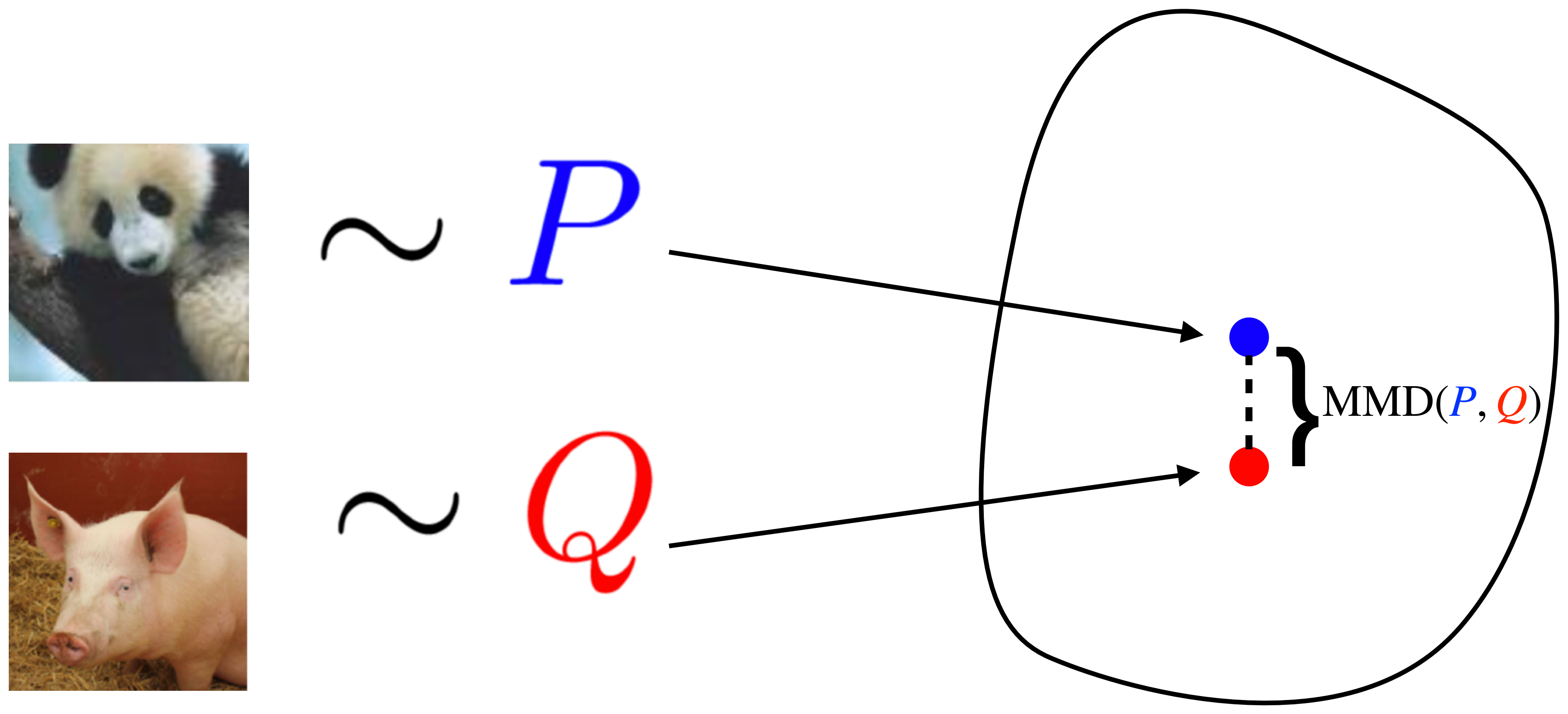
Dual formulation as an integral probability metric.

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

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



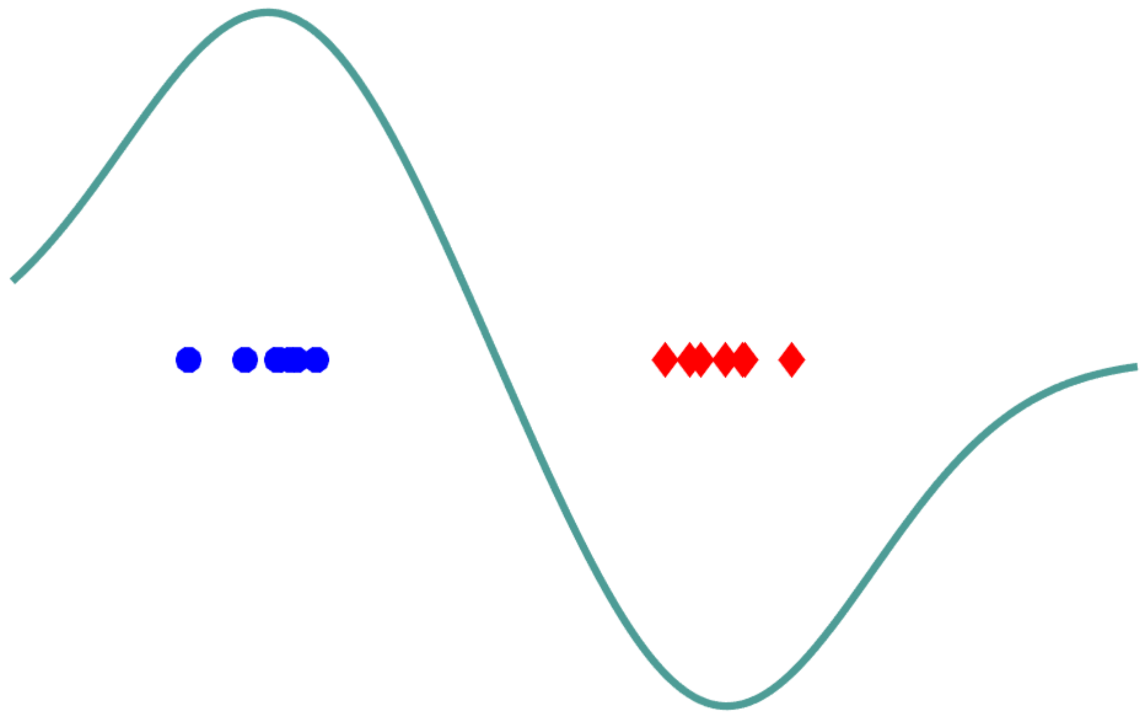


Figure credit: W. Jitkrittum, J. Zhu, H. Kremer

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

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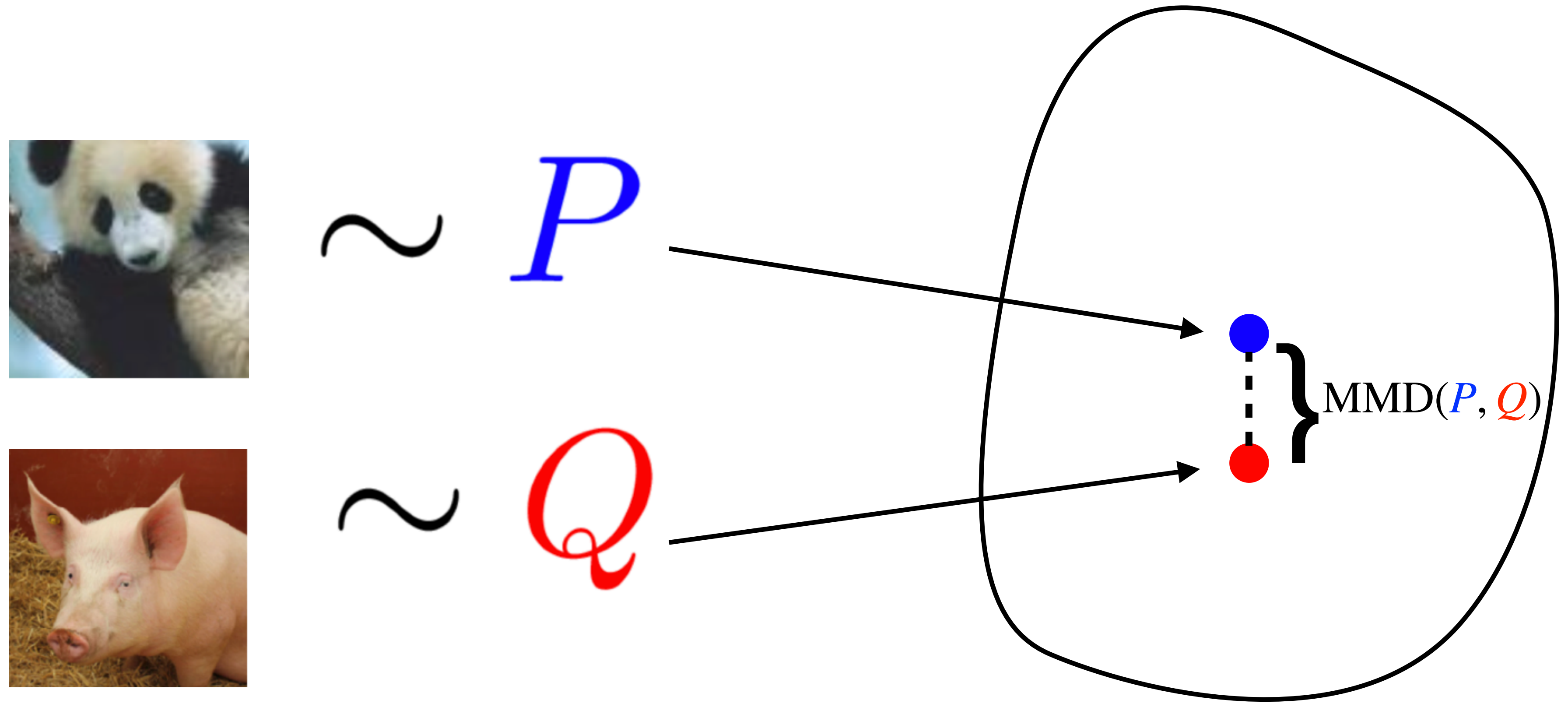
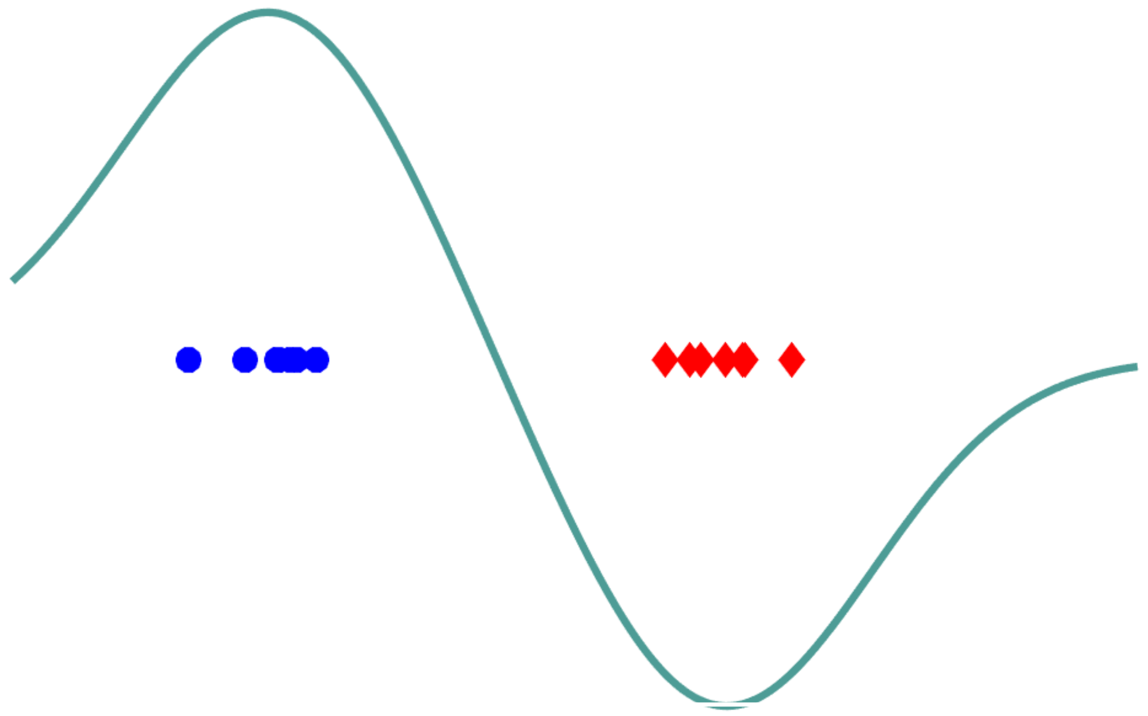
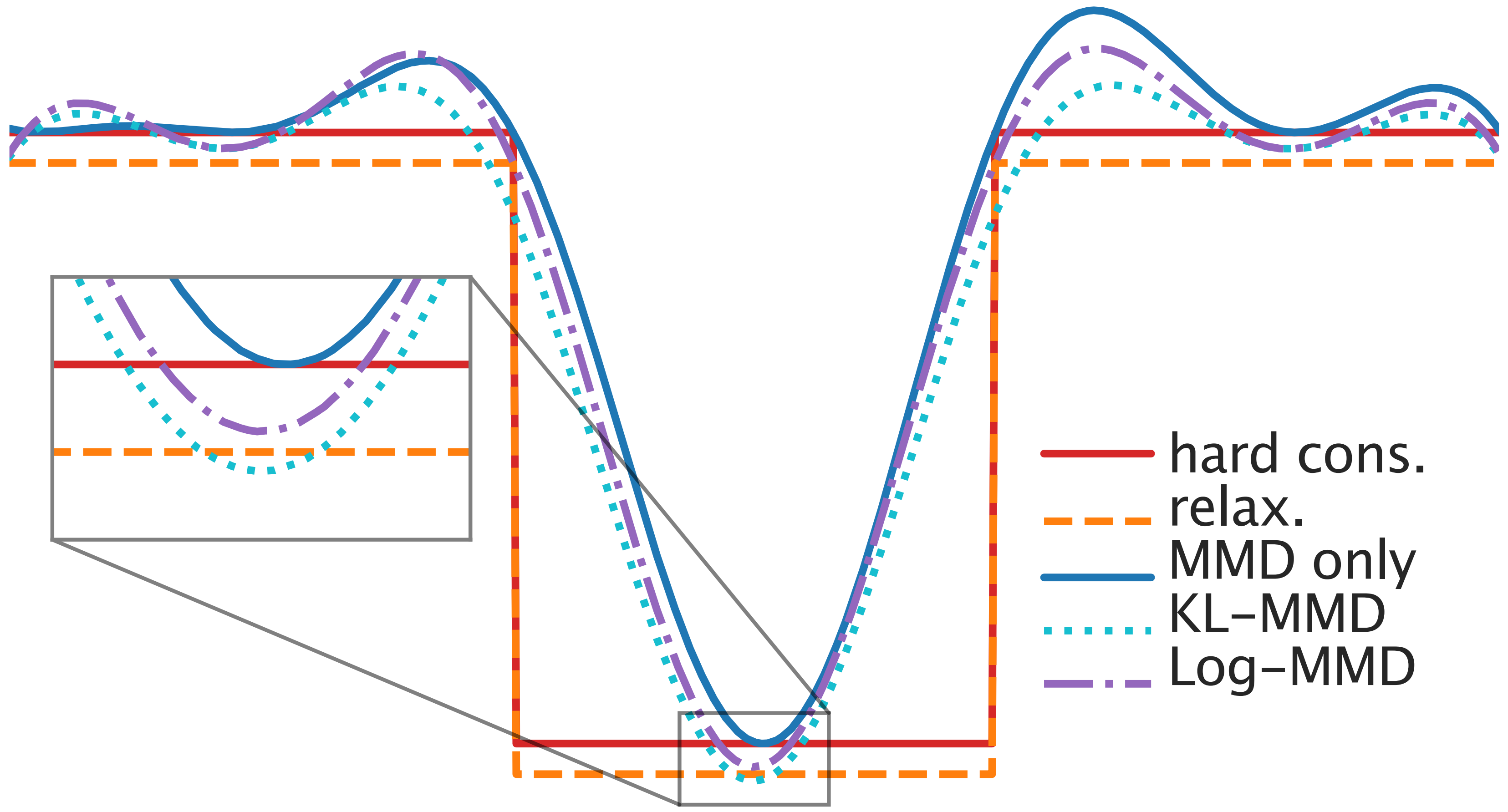
Duality leads to “interior point method” for prob. distributions







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Previous work: Kernel DRO

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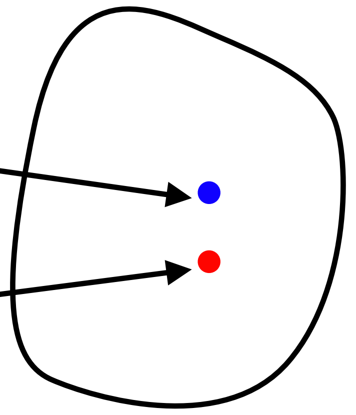
Primal DRO (not solvable as it is)

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

 $\sim P$

 $\sim Q$



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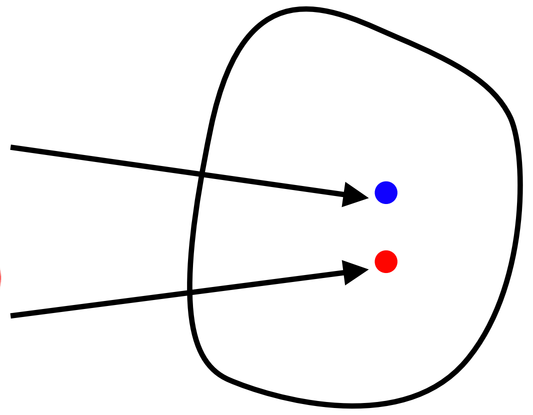

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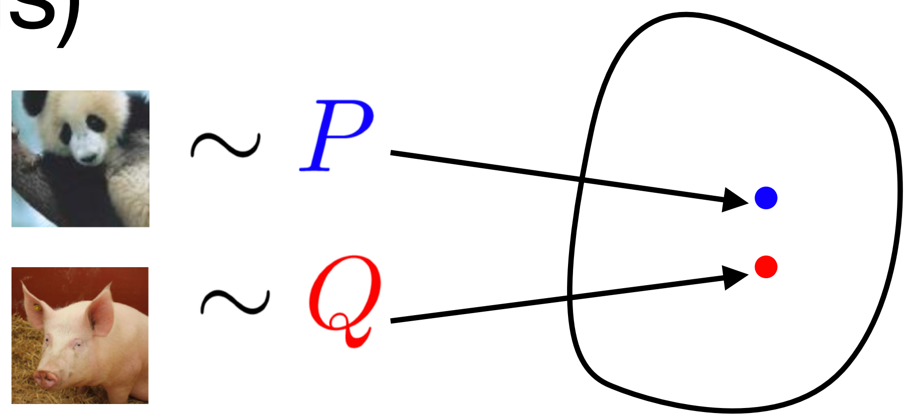

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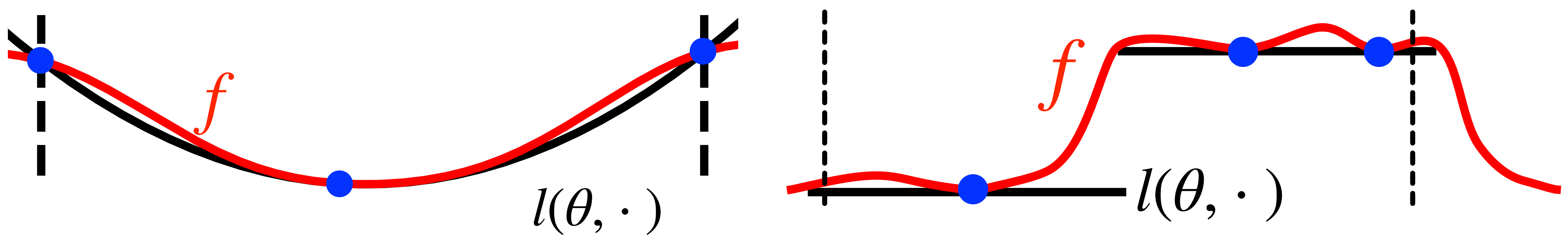

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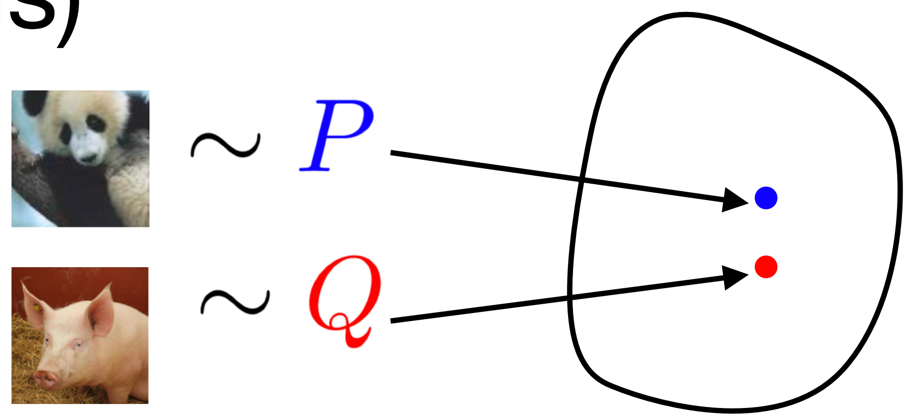

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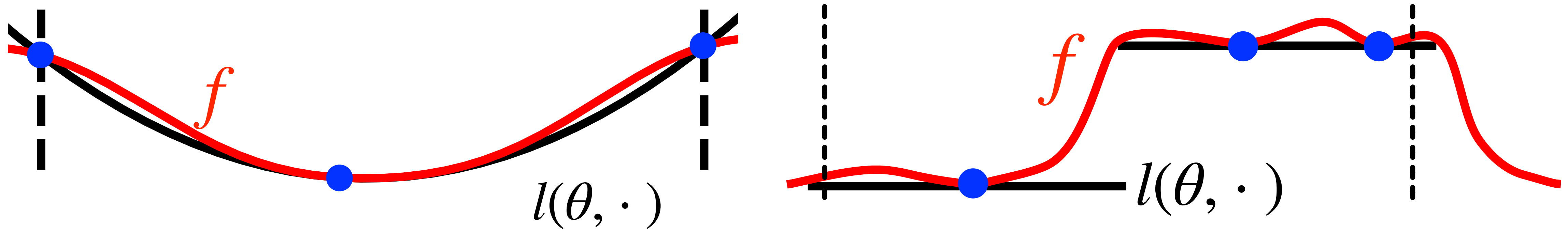

Example. Robust least squares

[El Ghaoui Lebret '97]

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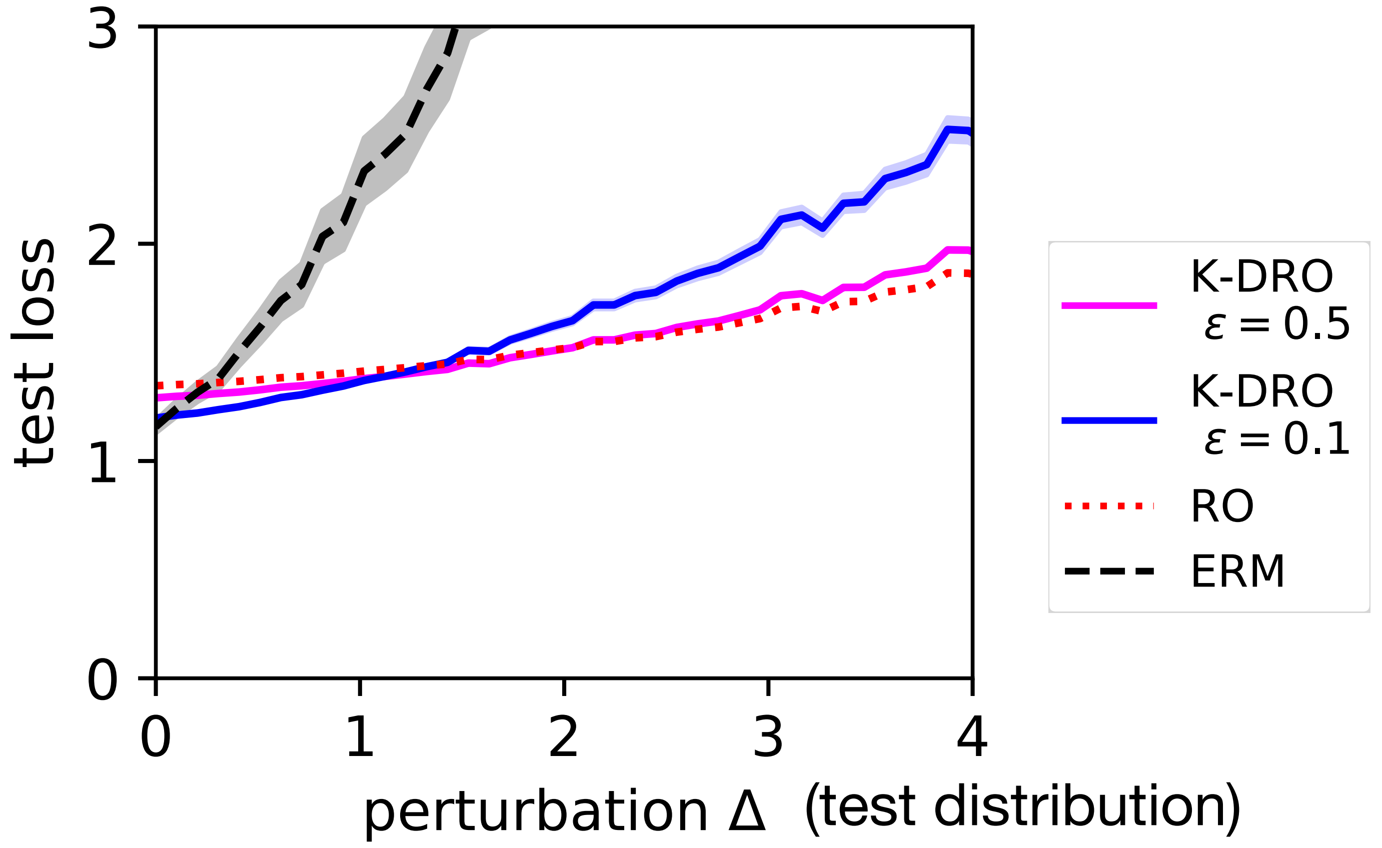
Given historical samples $\xi_1, \xi_2, \ldots, \xi_N$



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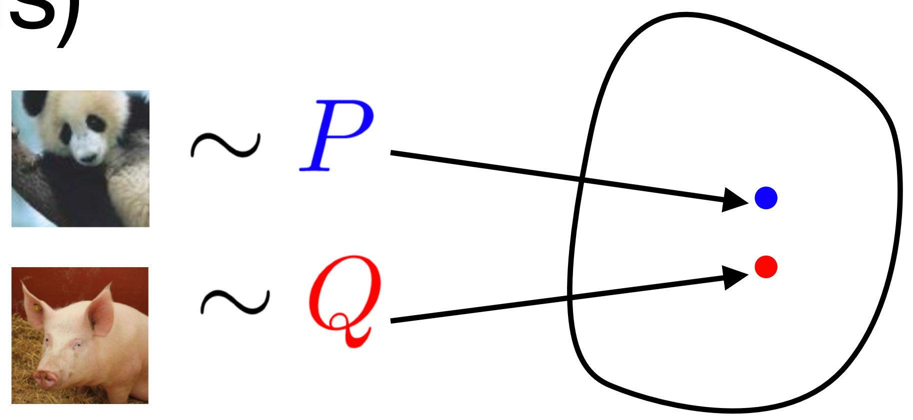

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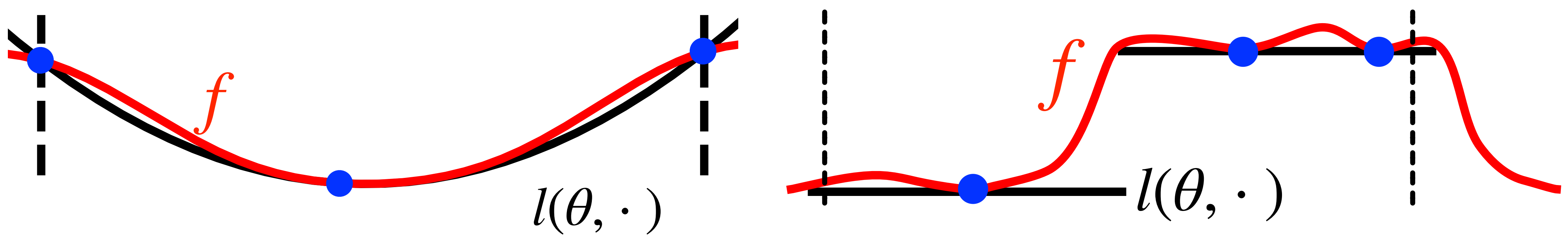

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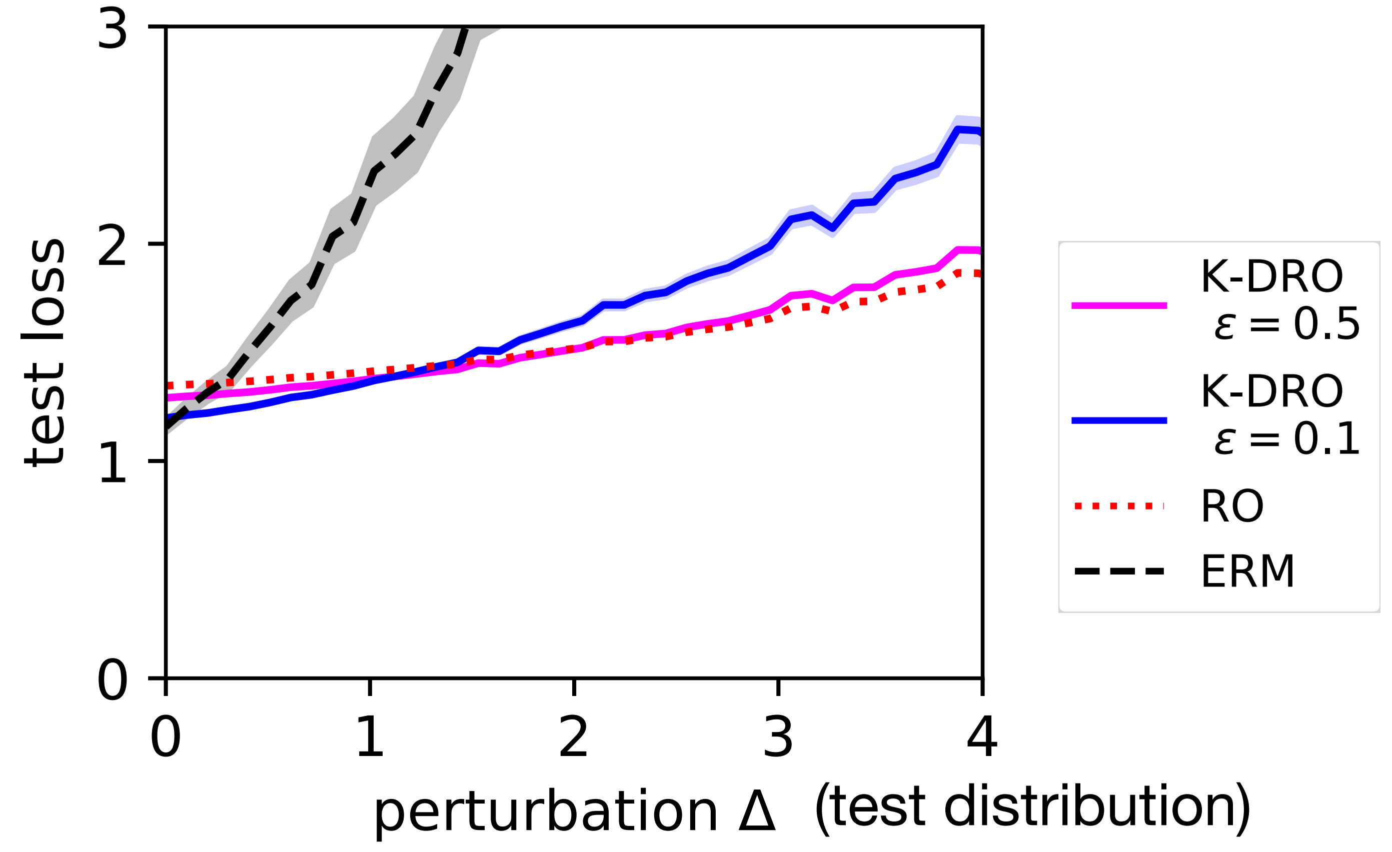
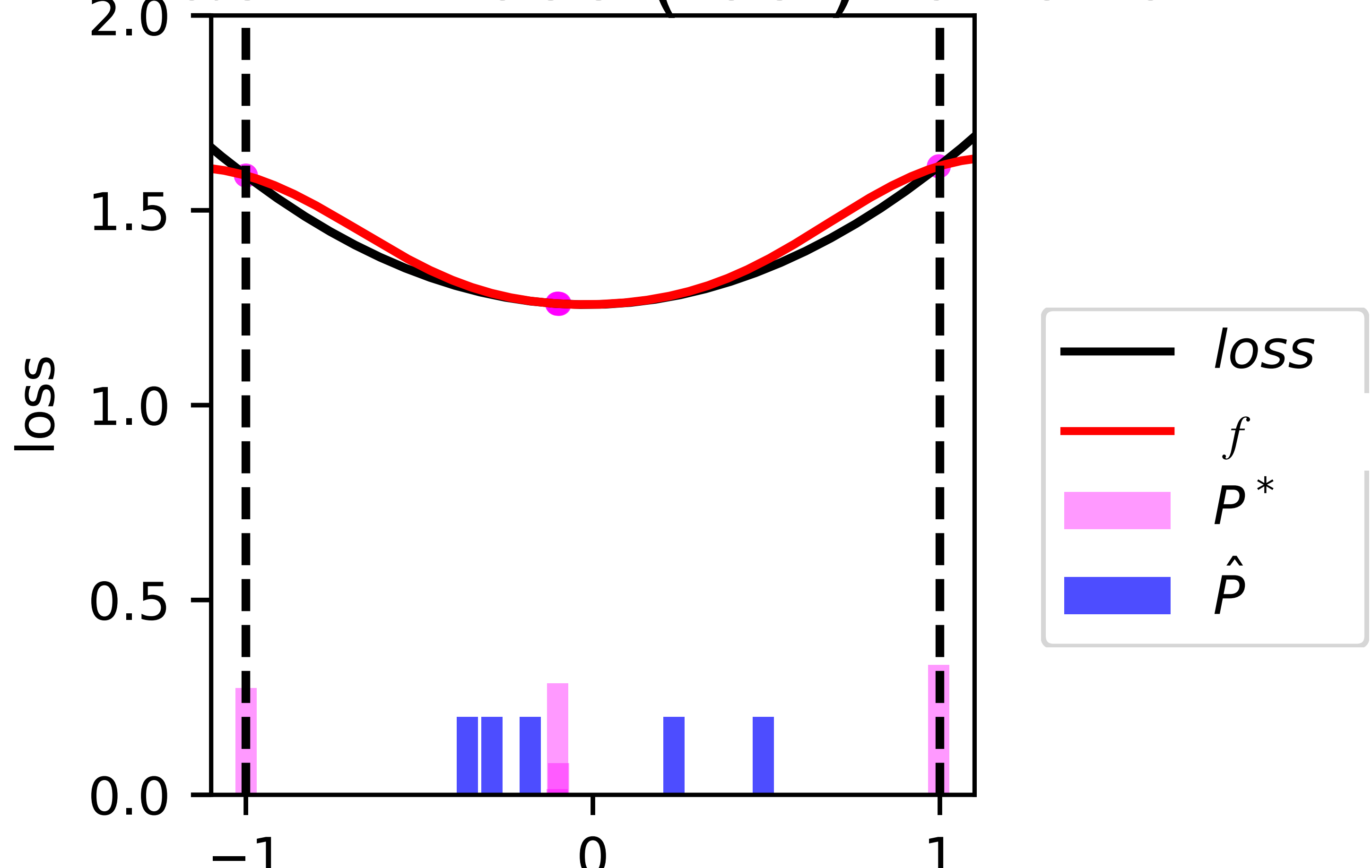


Robustifying with DRO

f as witness (test) function



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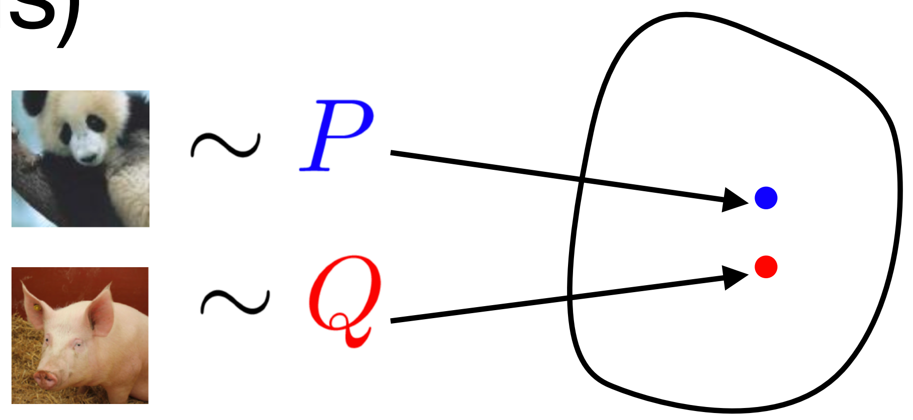

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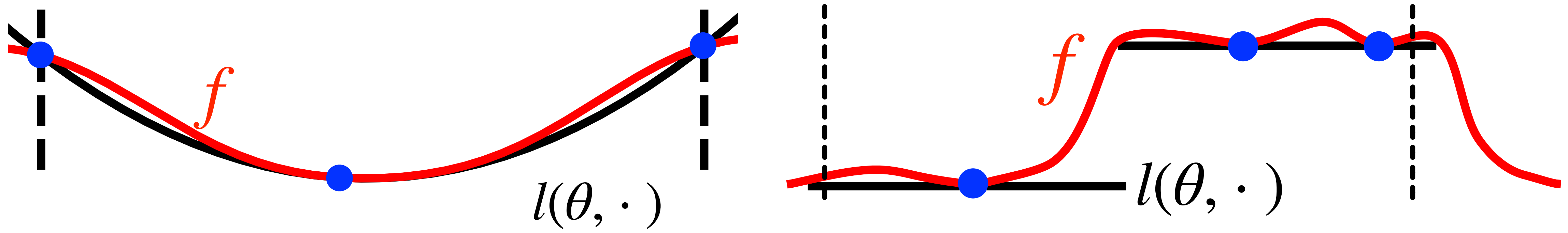

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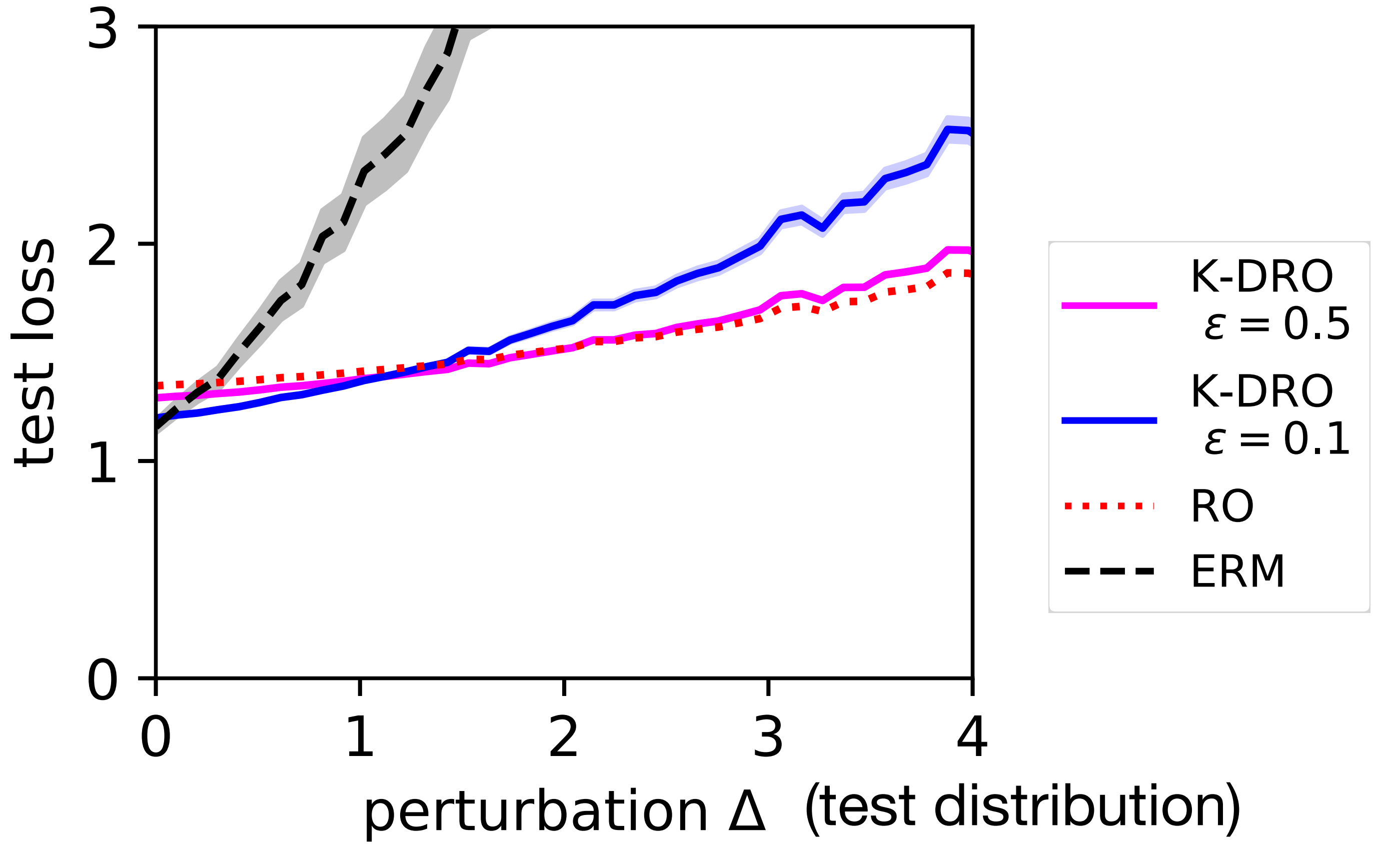

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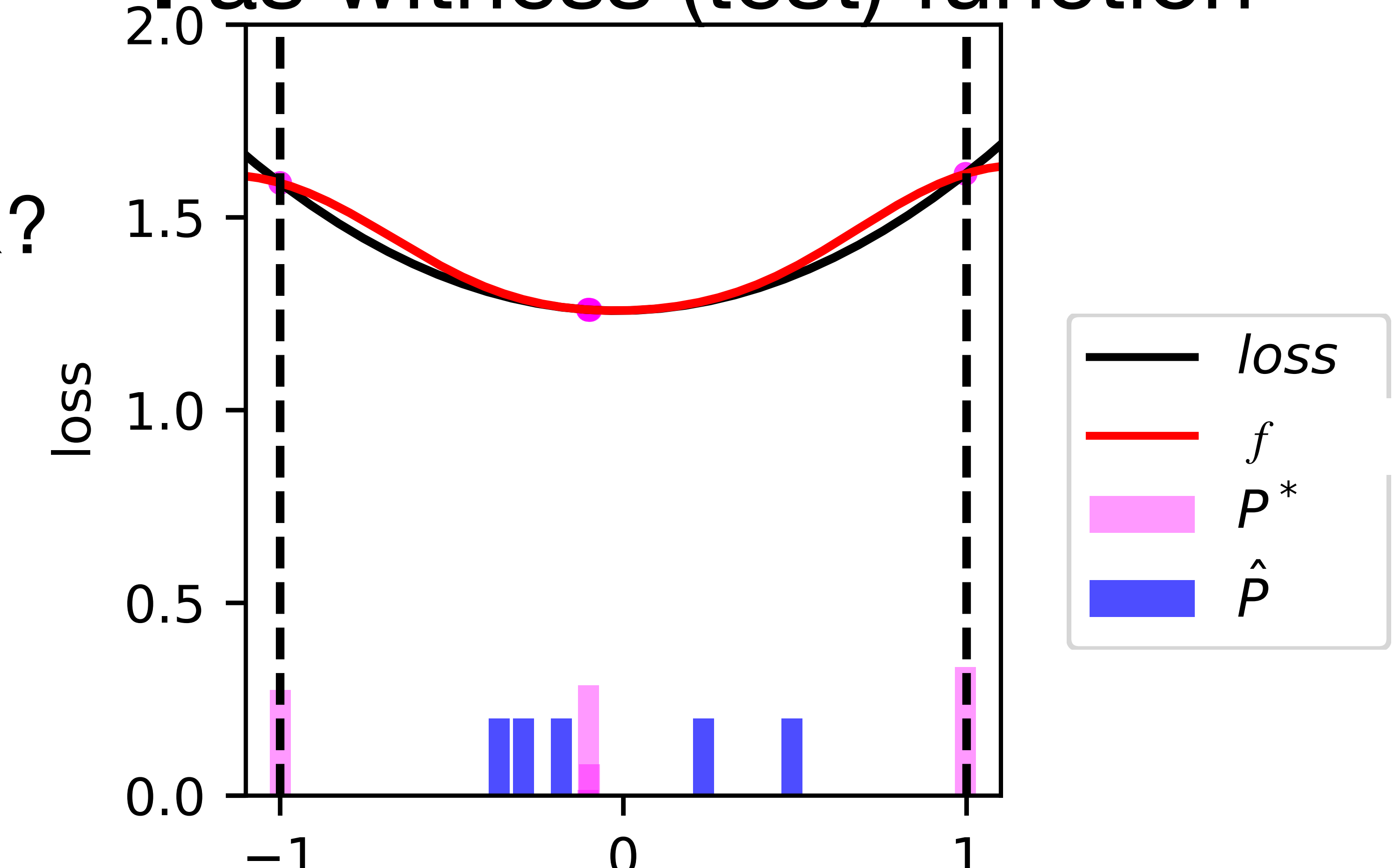

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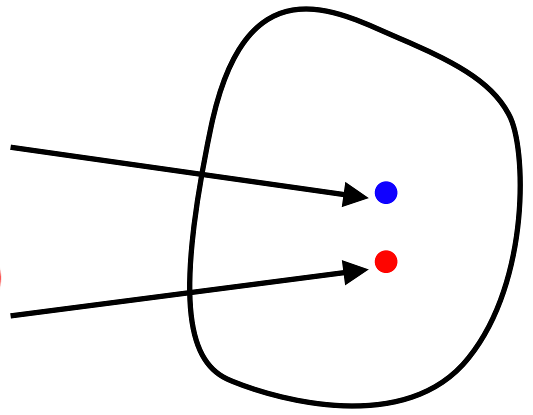

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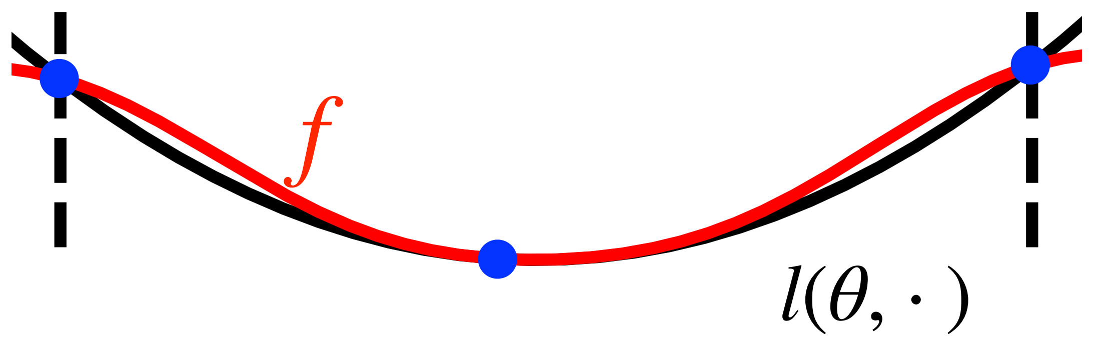

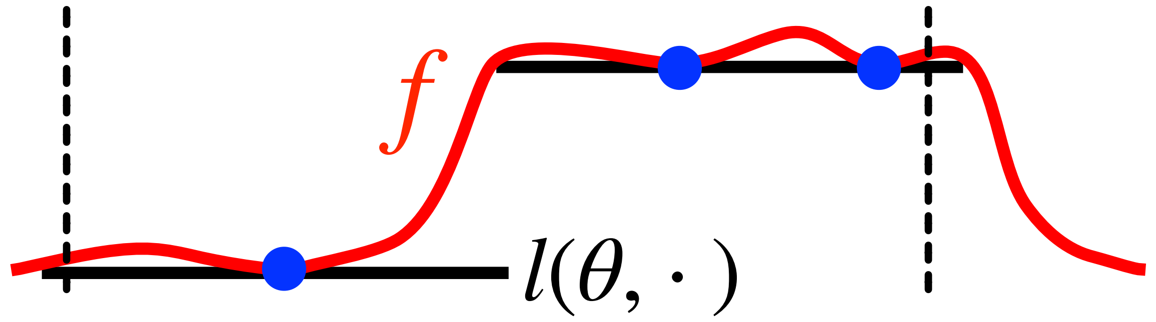

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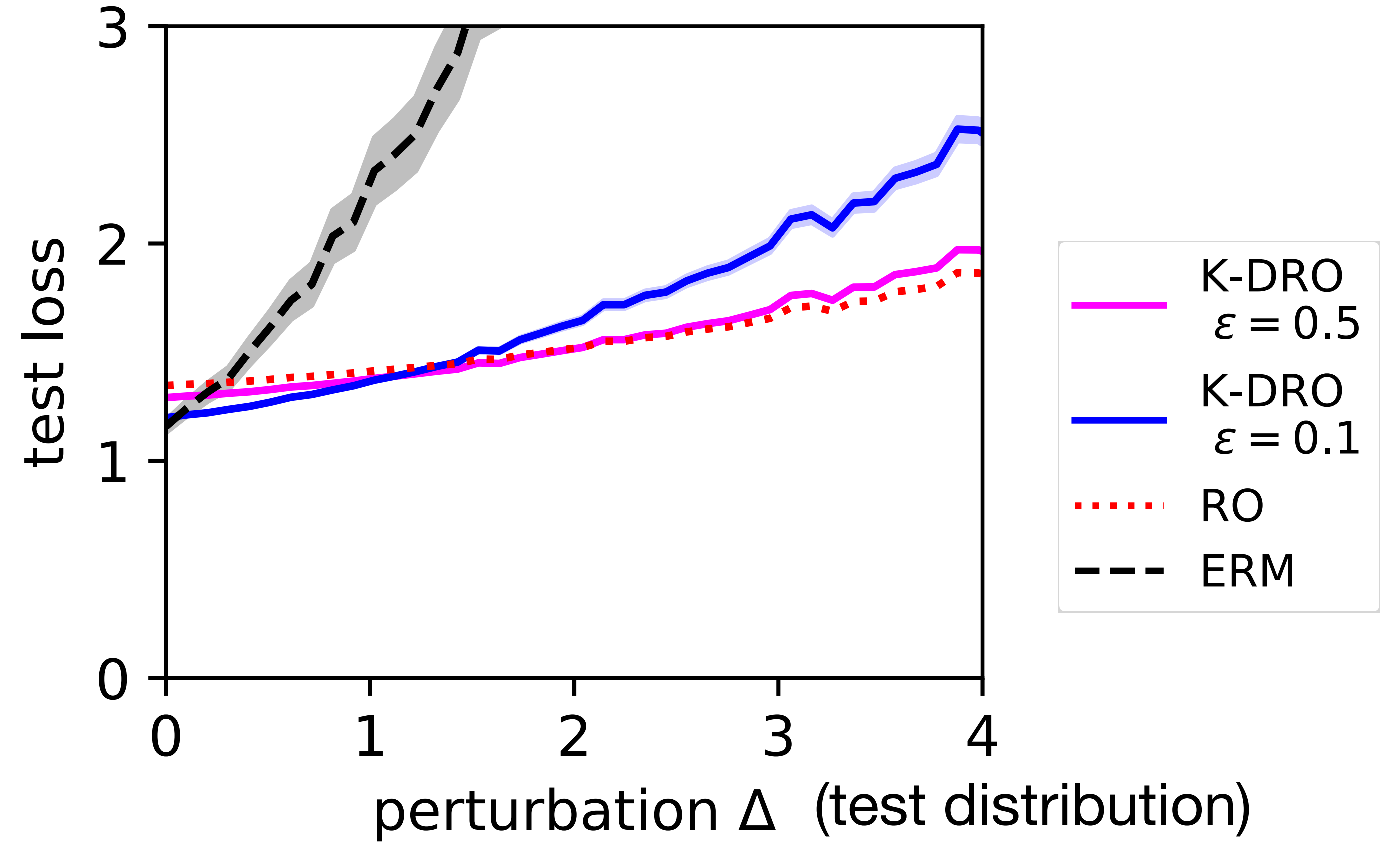

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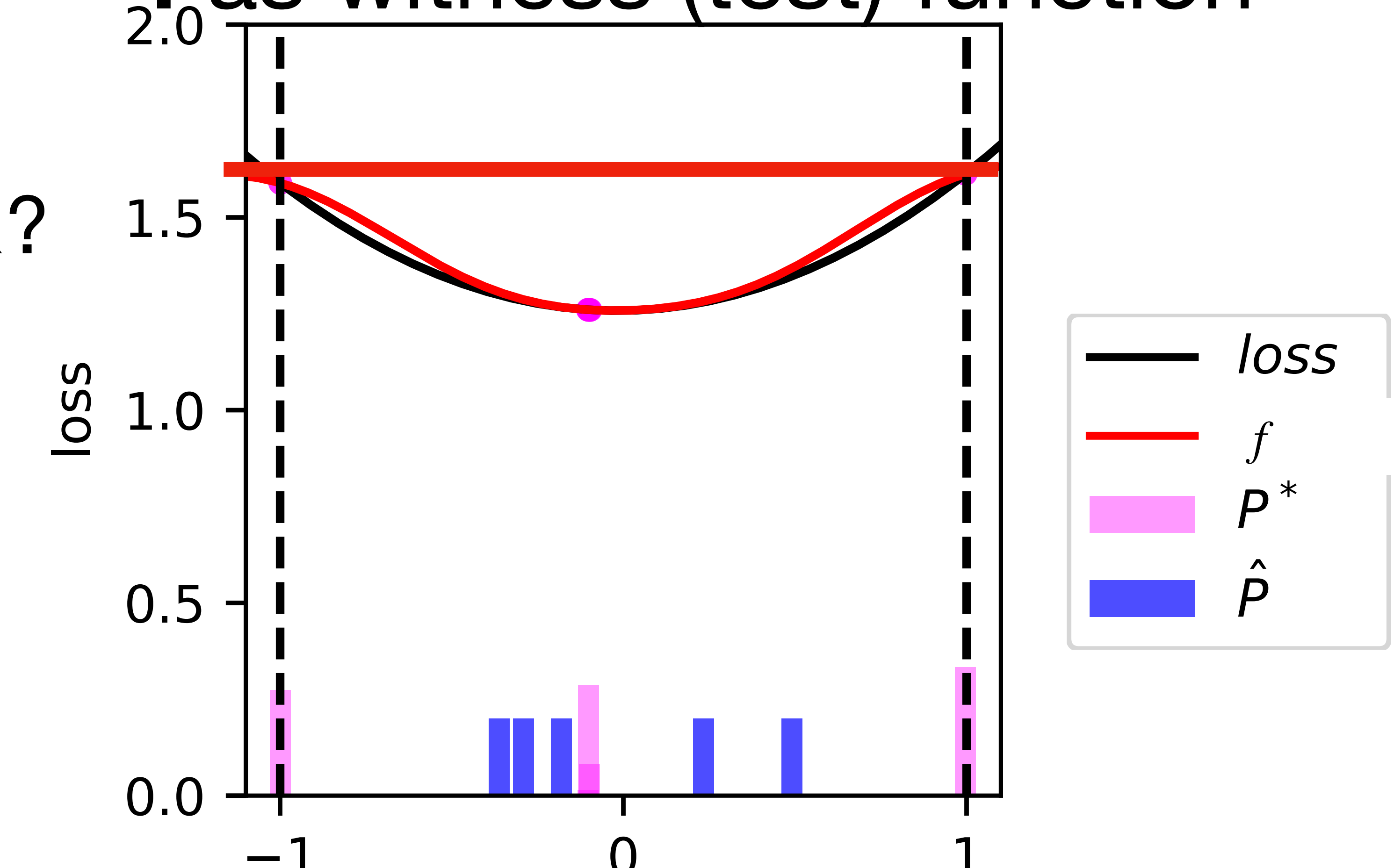

Duality perspective

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2-Wasserstein

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

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

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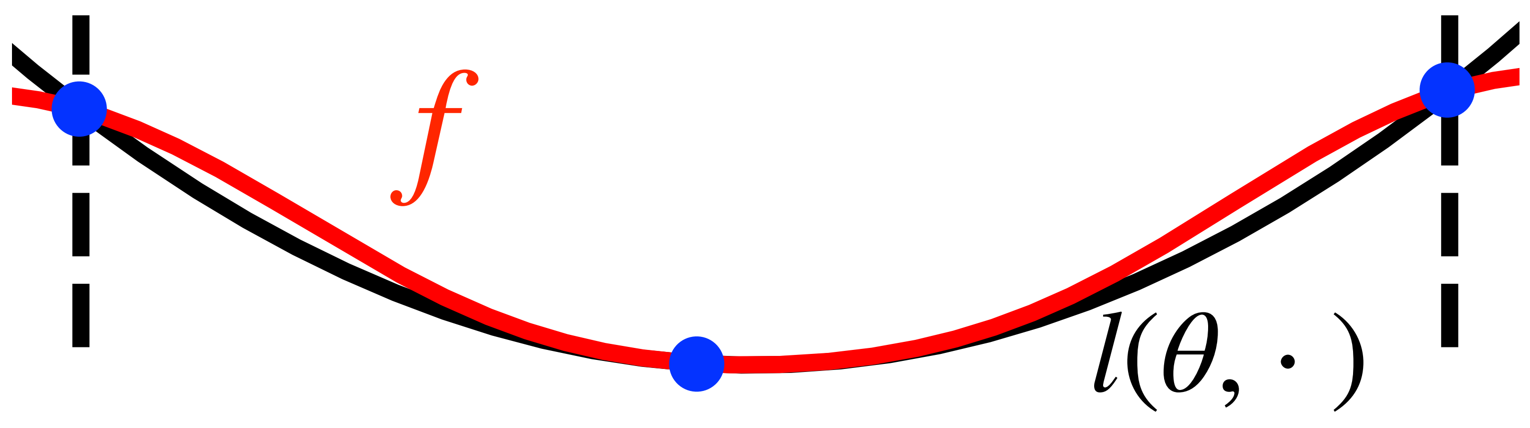

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- l is **nonconvex** (e.g., DNN, g-non-cvx)
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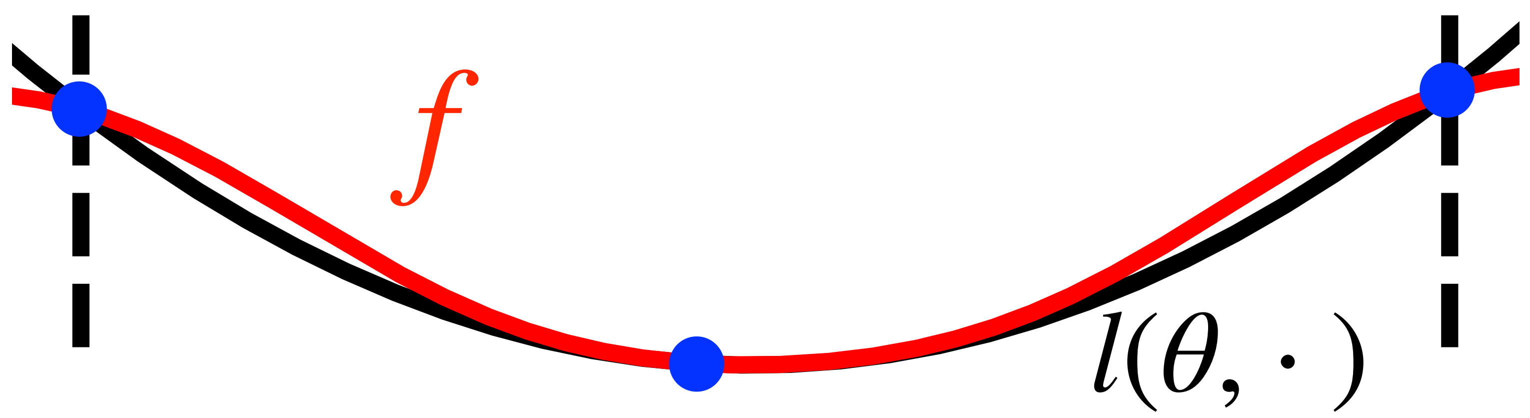

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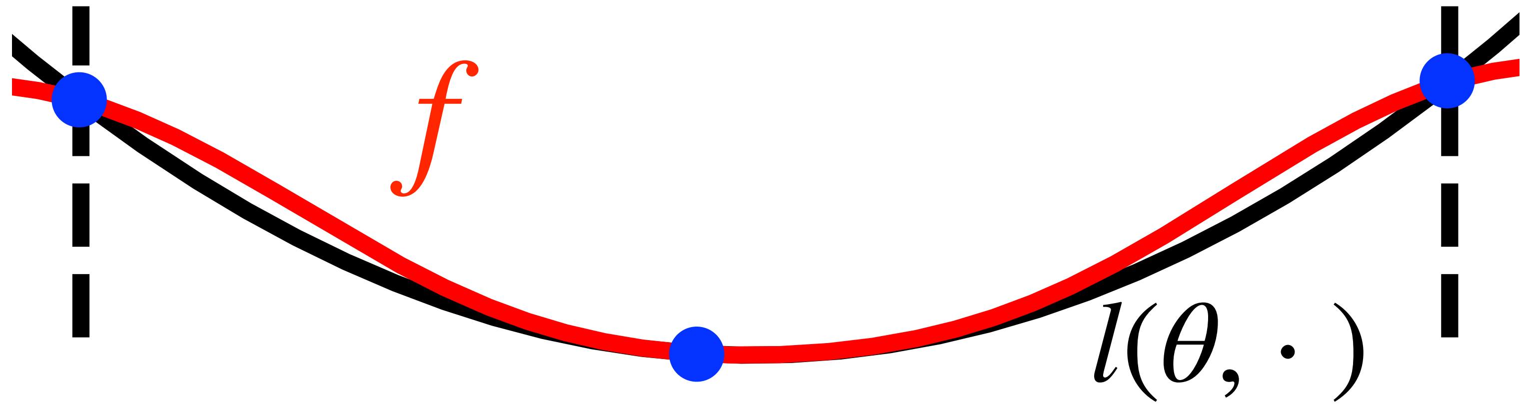

Nonlinear kernel approx. as robust surrogate losses (flatten the curve)

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

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

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

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

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

Duality in gradient flow dynamics: nonlinear ODE

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

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

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

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

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

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.

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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]

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

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