Duality from Distributionally Robust Learning to Gradient Flow Force-Balance

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Weierstraß-Institut für
Angewandte Analysis und Stochastik

Duality of
Distributionally Robust Learning

Distributional **robustness**, but what kind?

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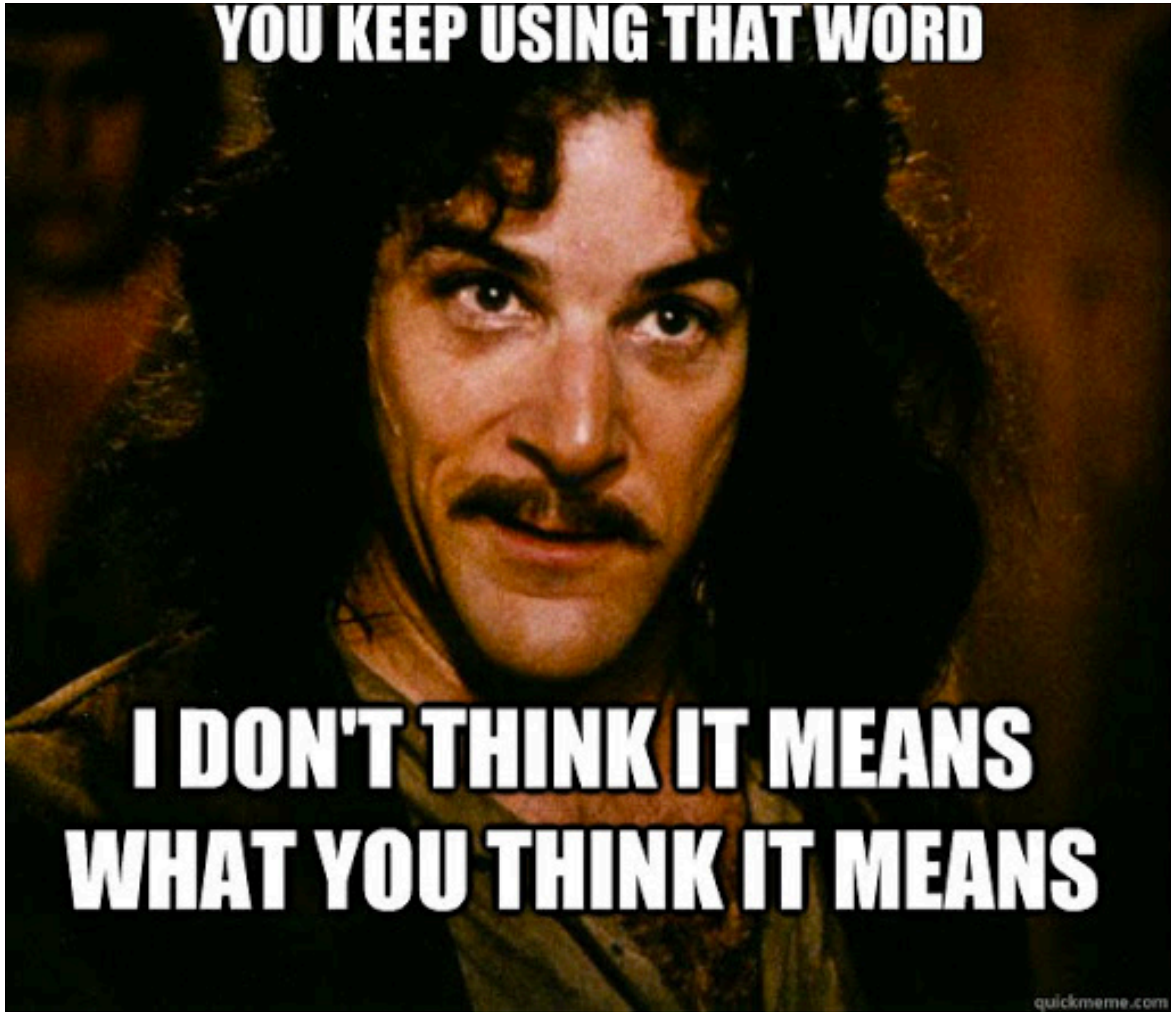

Figure credit: The Princess Bride,
a bedside story by your grandpa

From Statistical Learning to Distributionally Robust Learning

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

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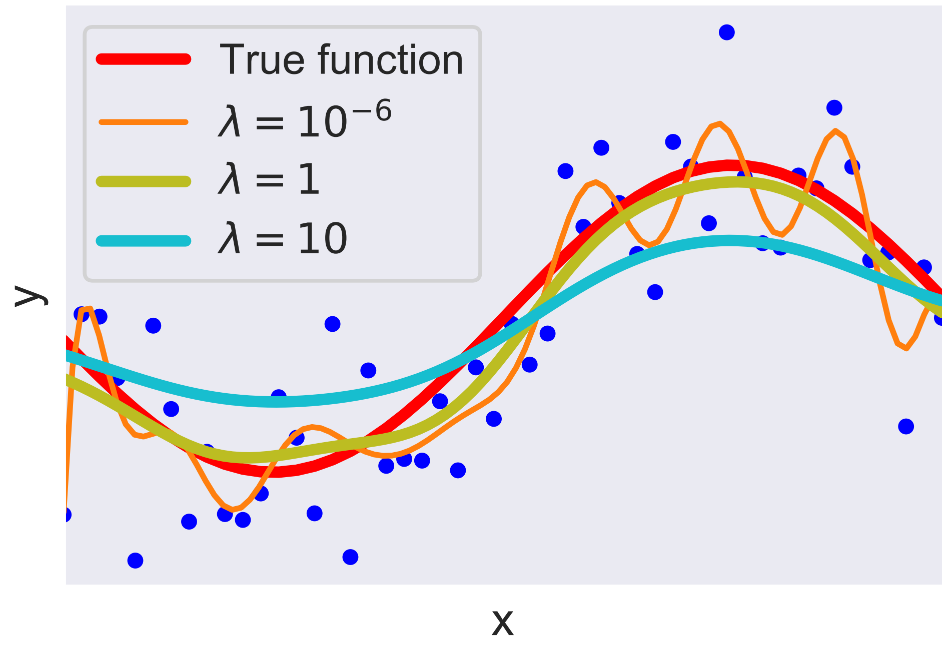

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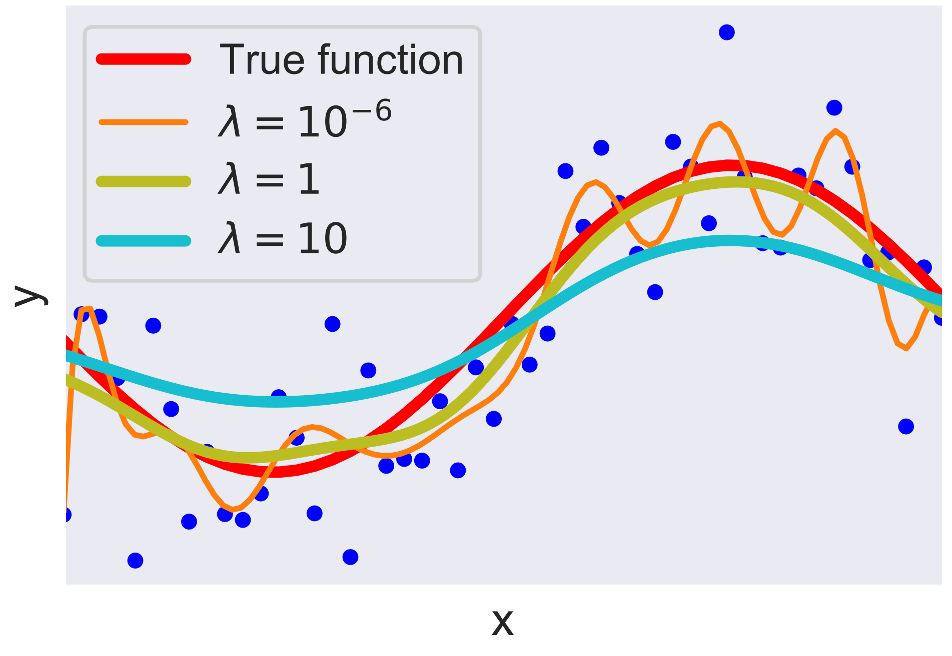

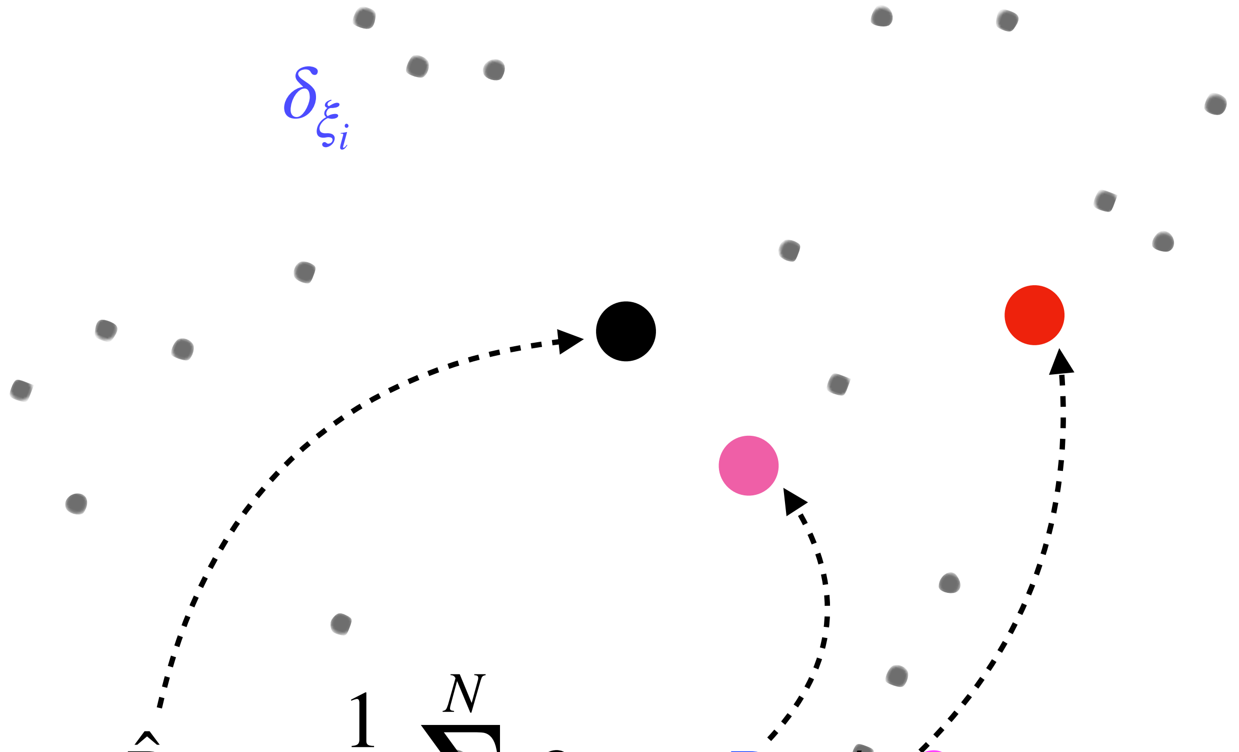

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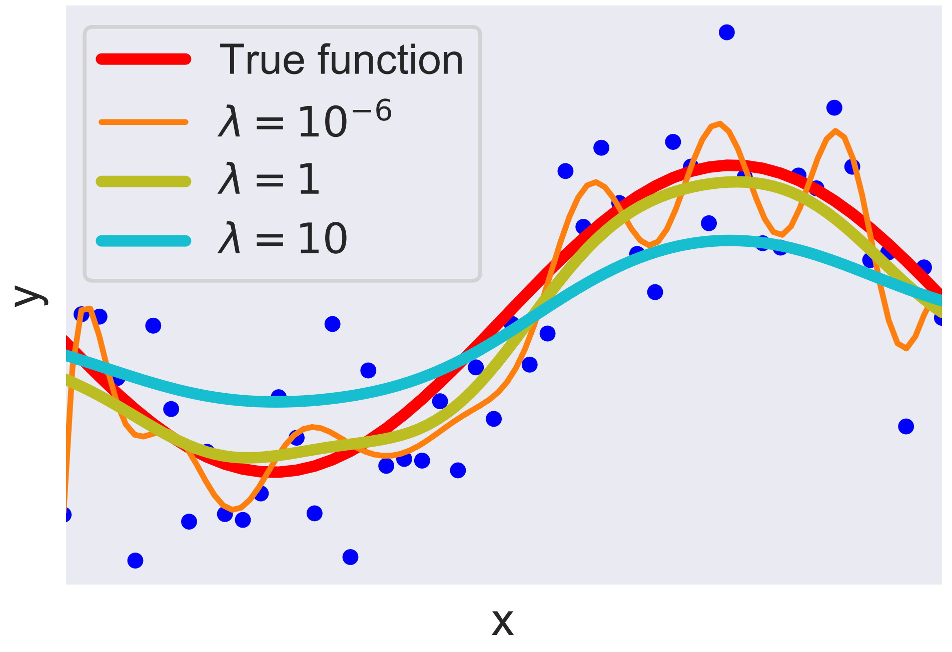

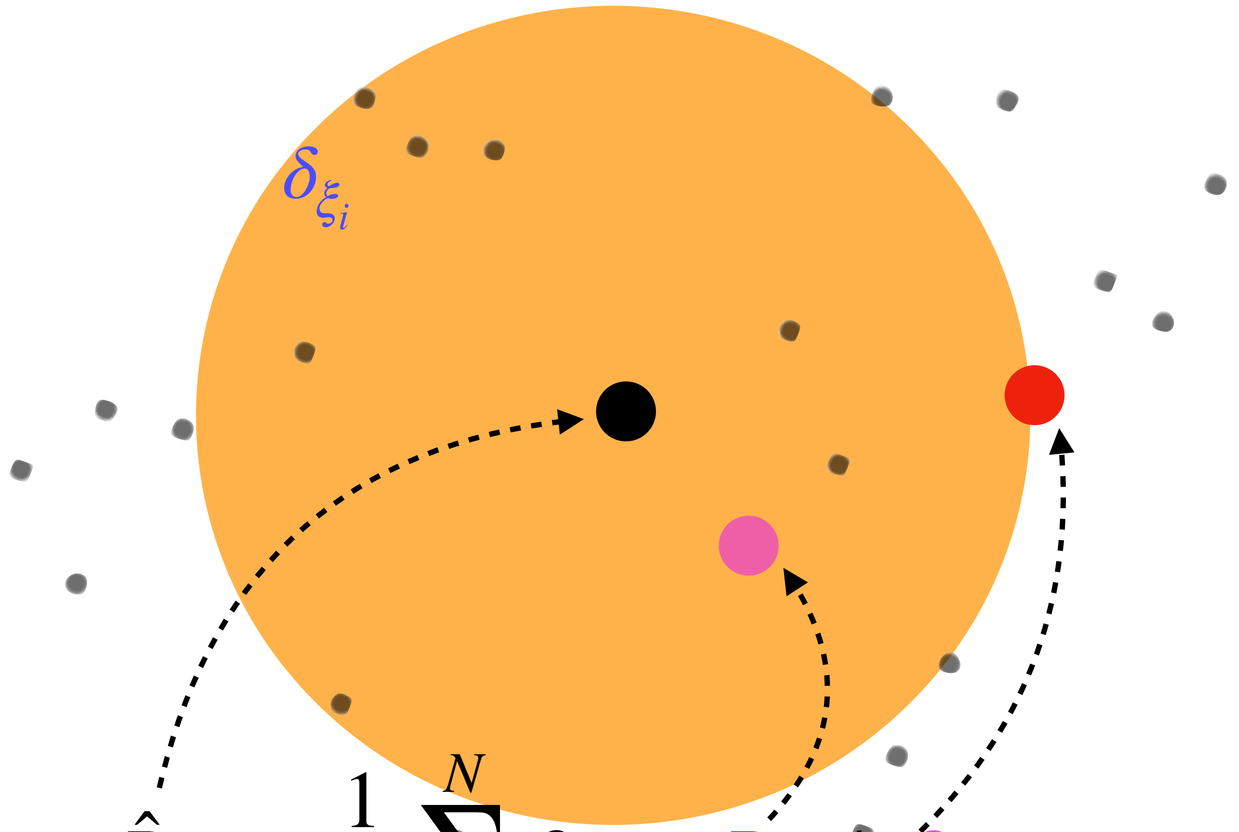

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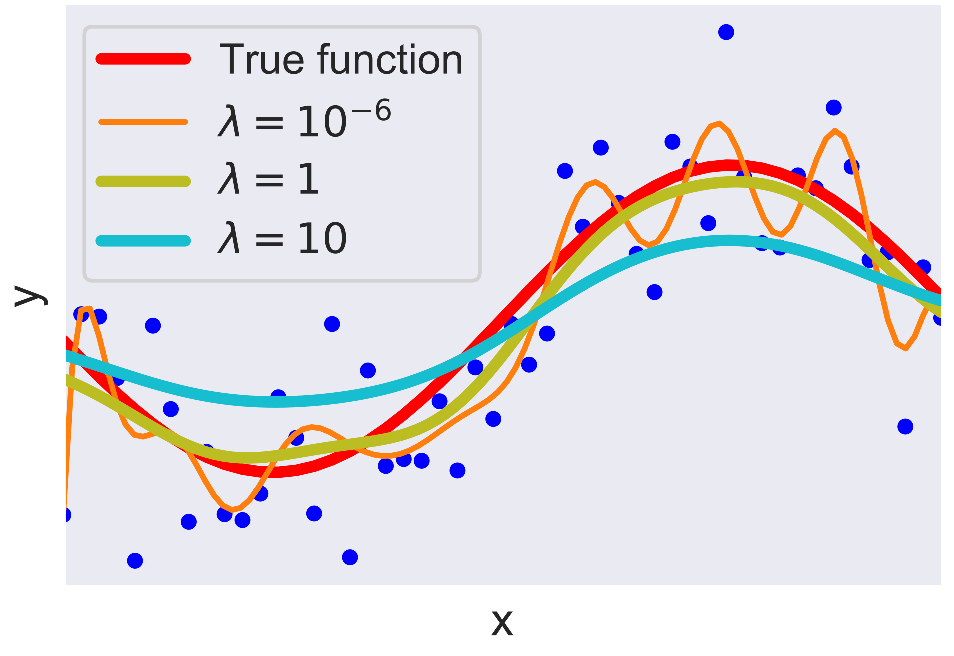

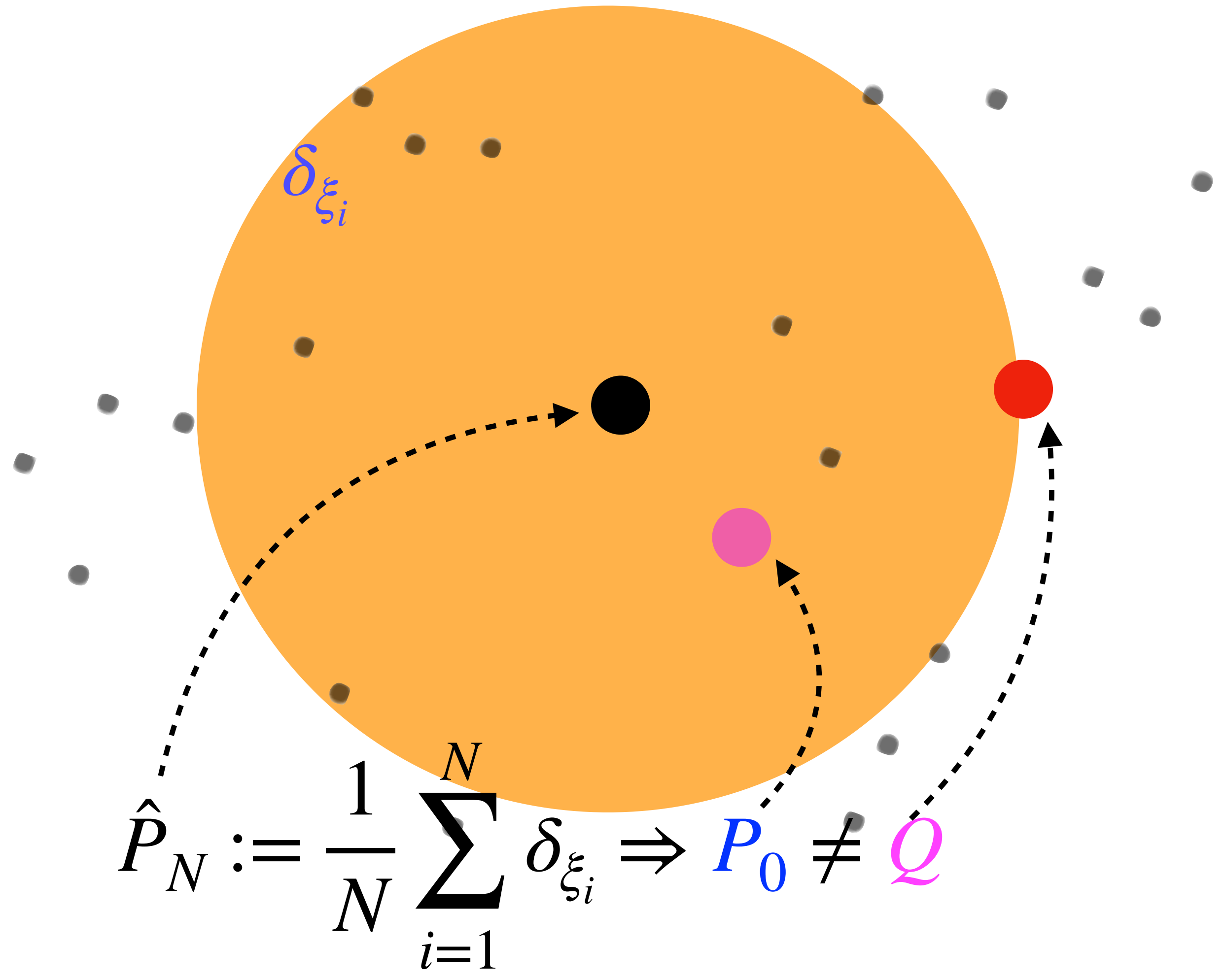

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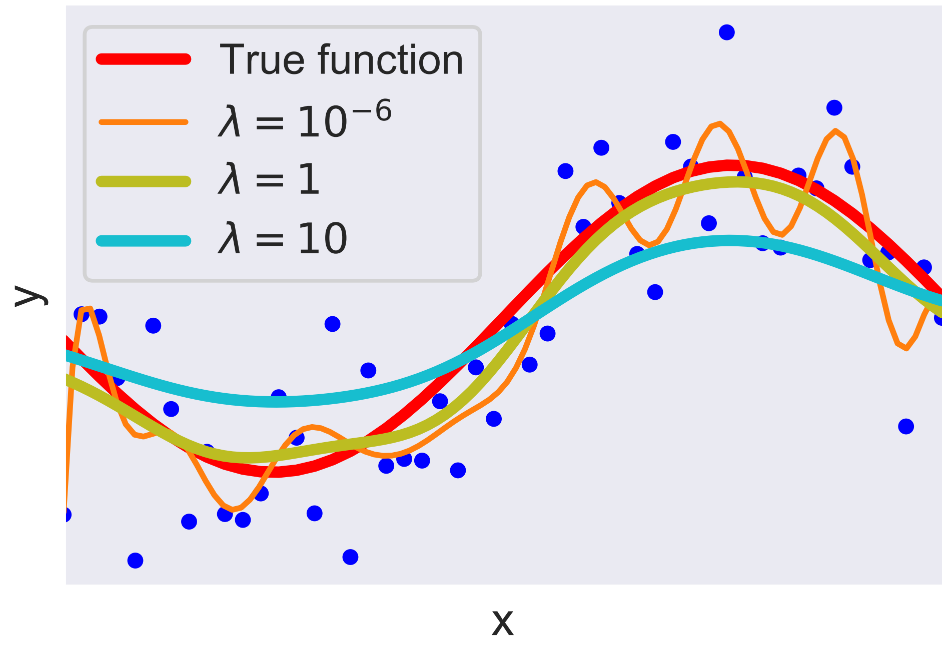

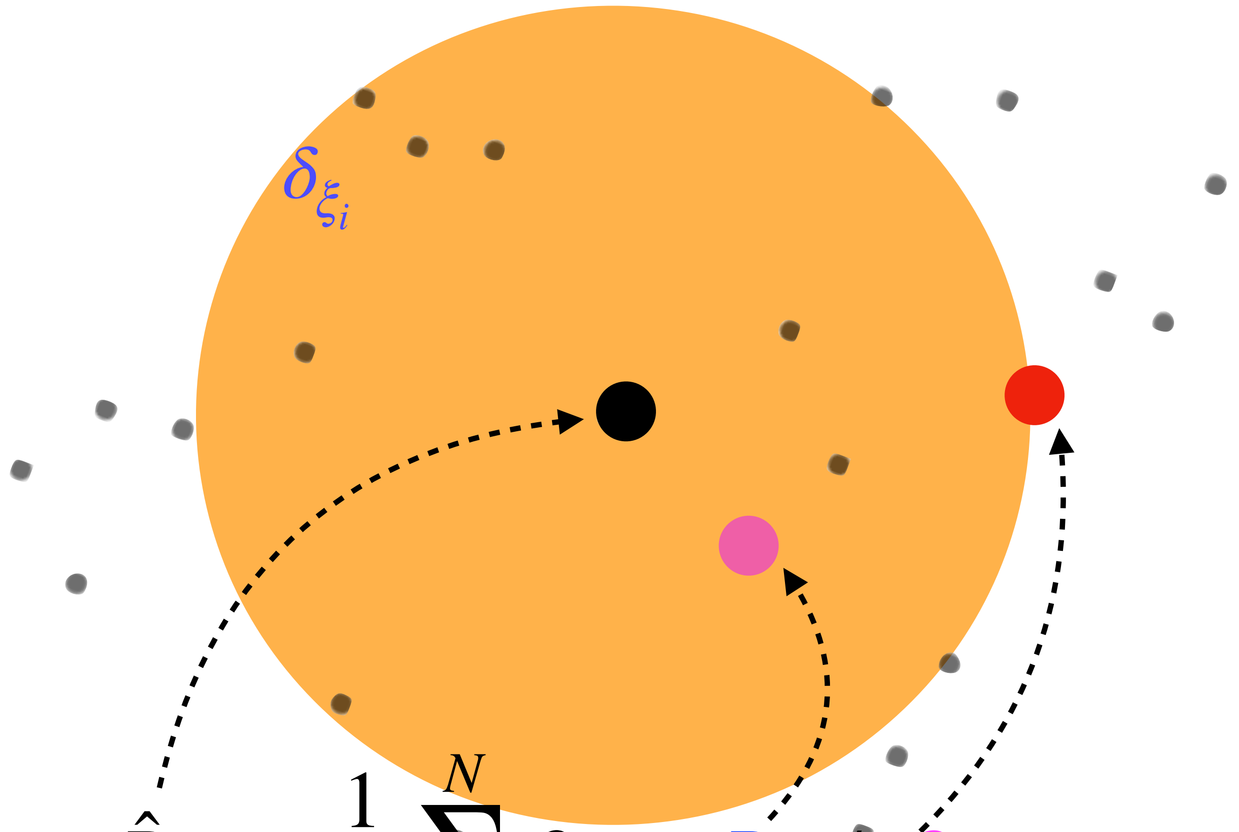

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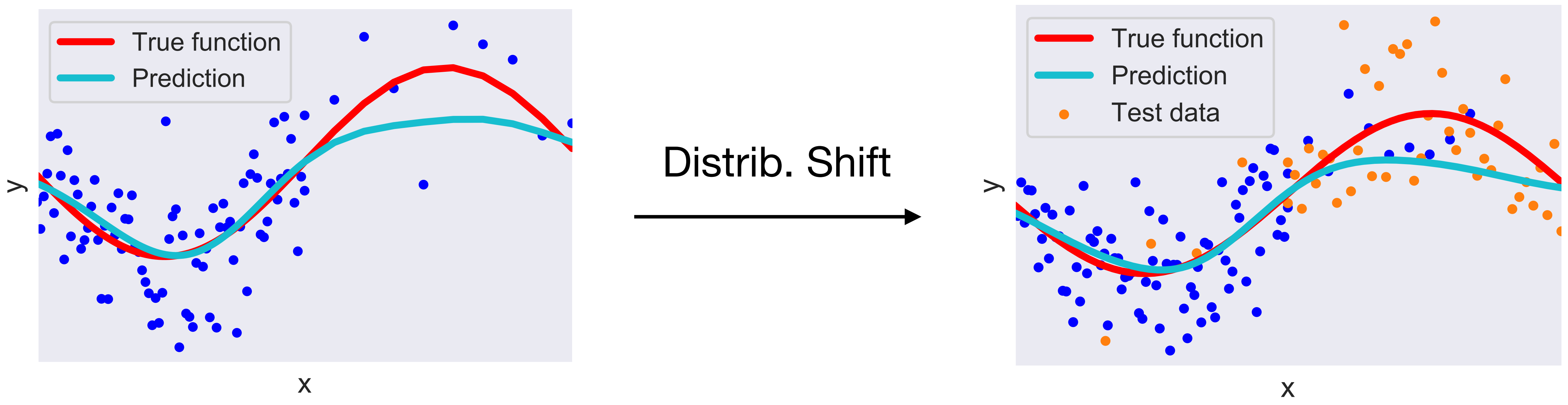

Figure credit: Heiner Kremer

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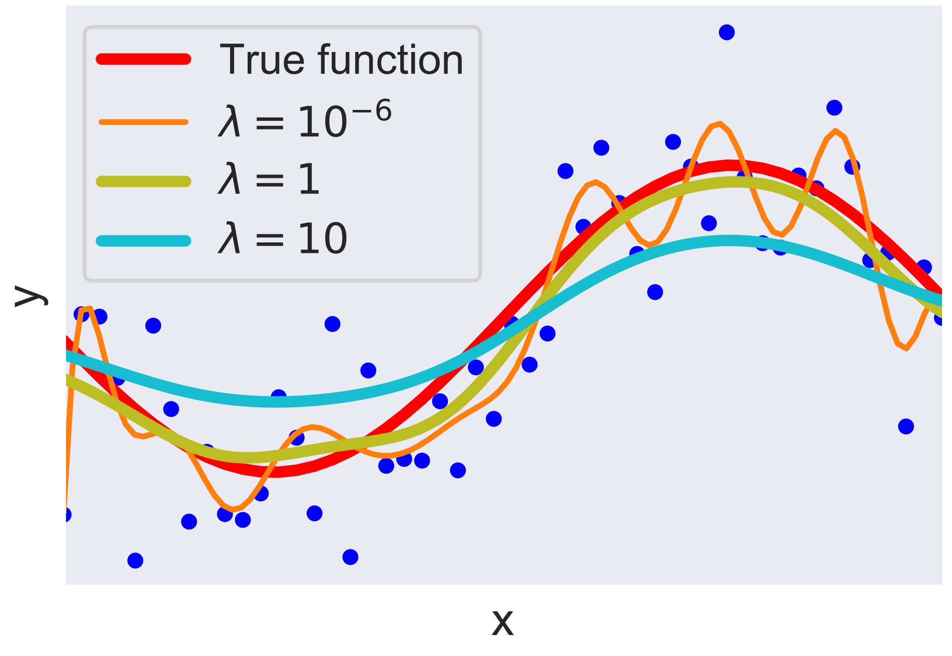

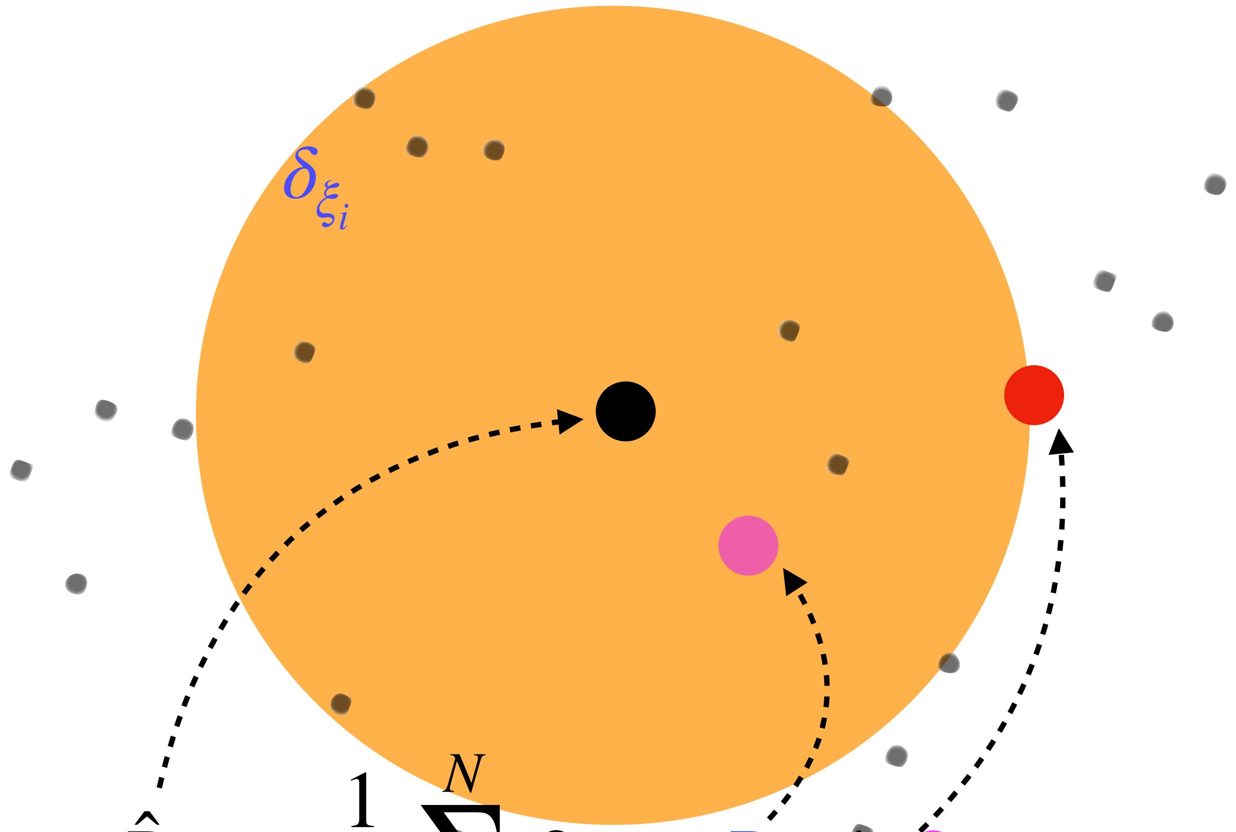

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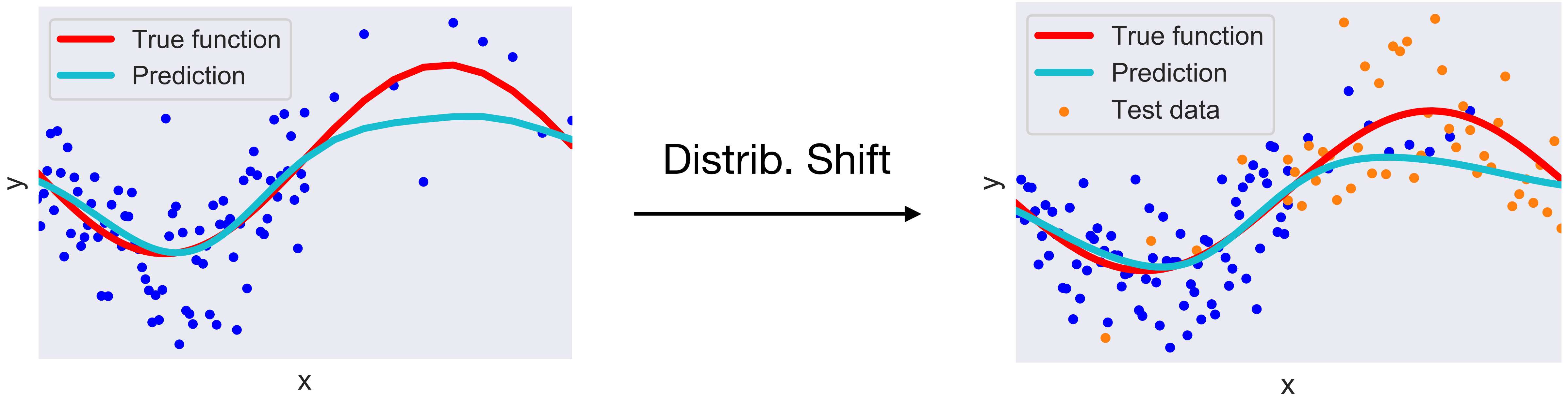

Why study new geometry?

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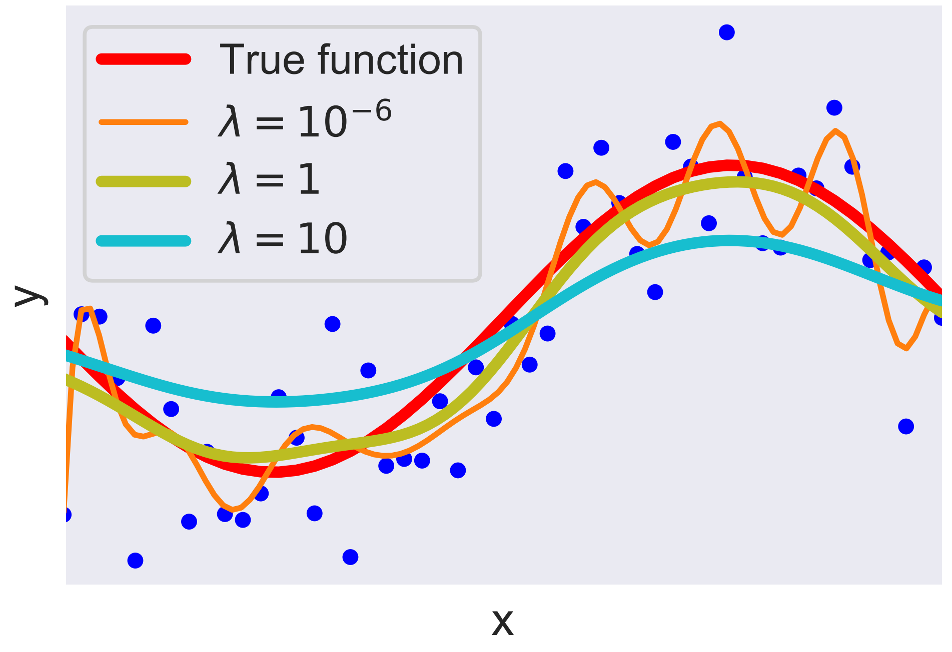

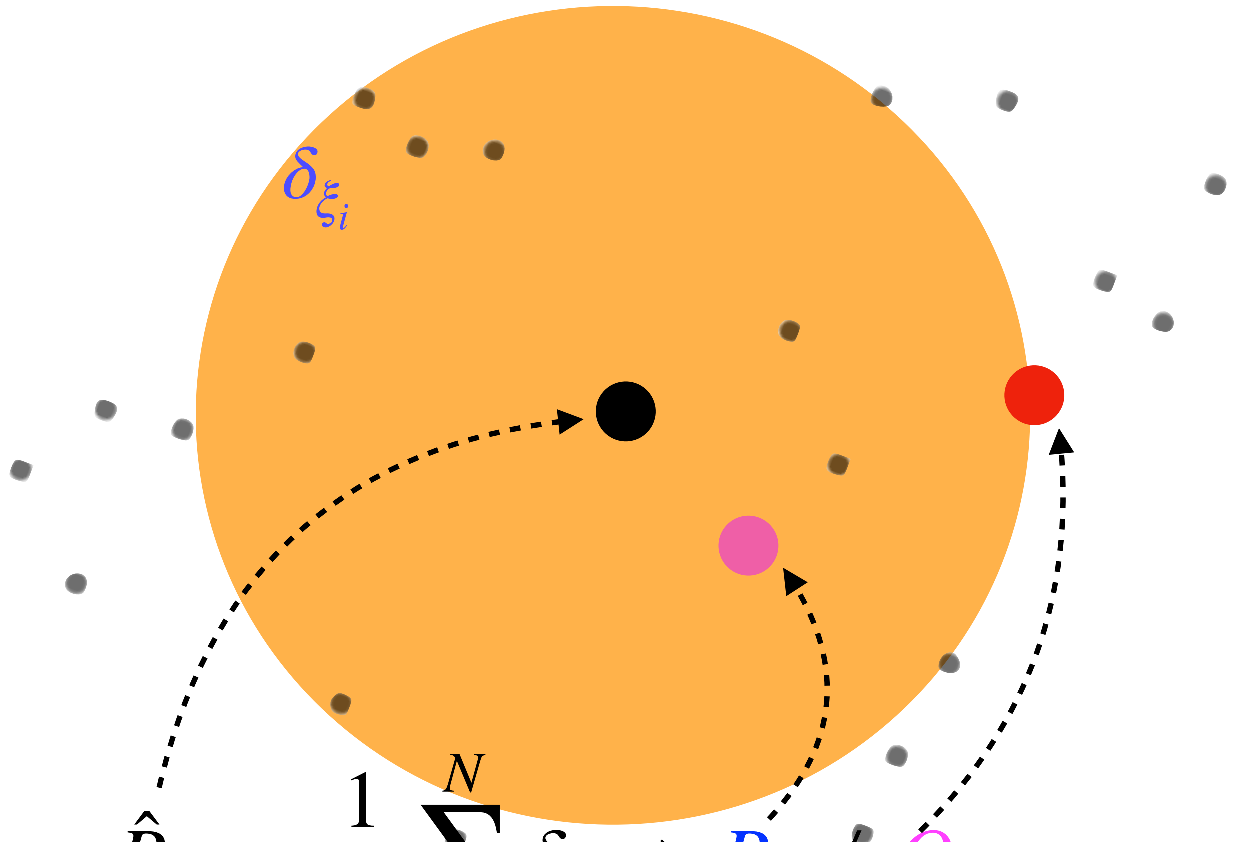

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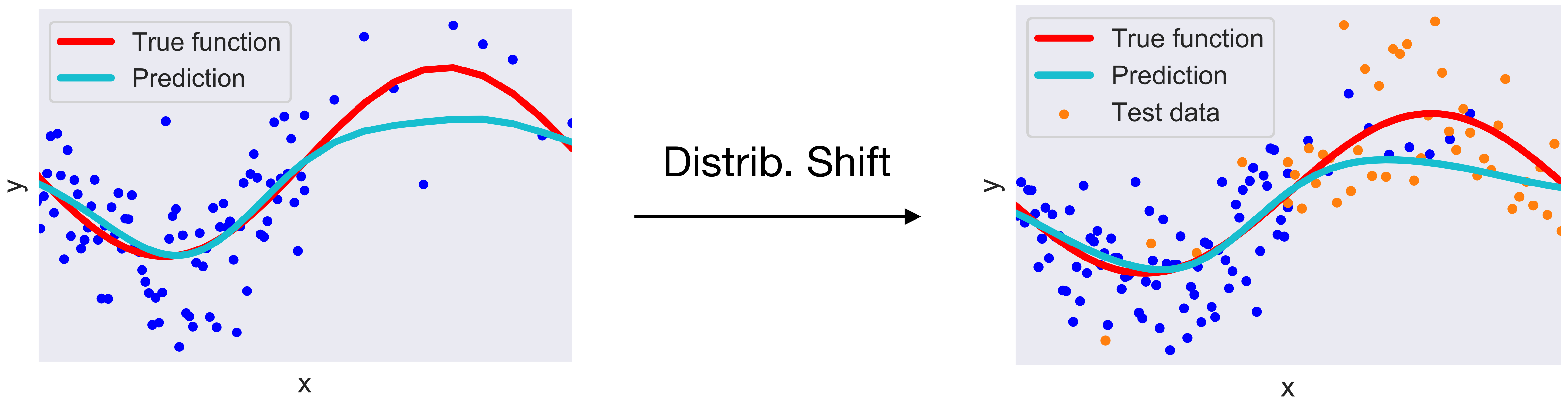

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New geometries leading to new fields of research and breakthroughs:

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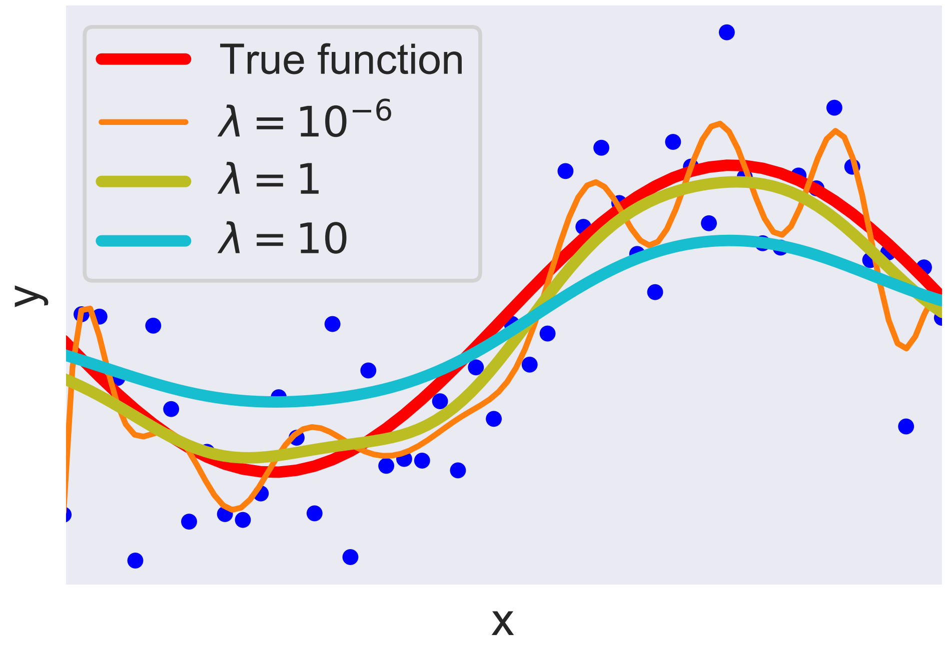

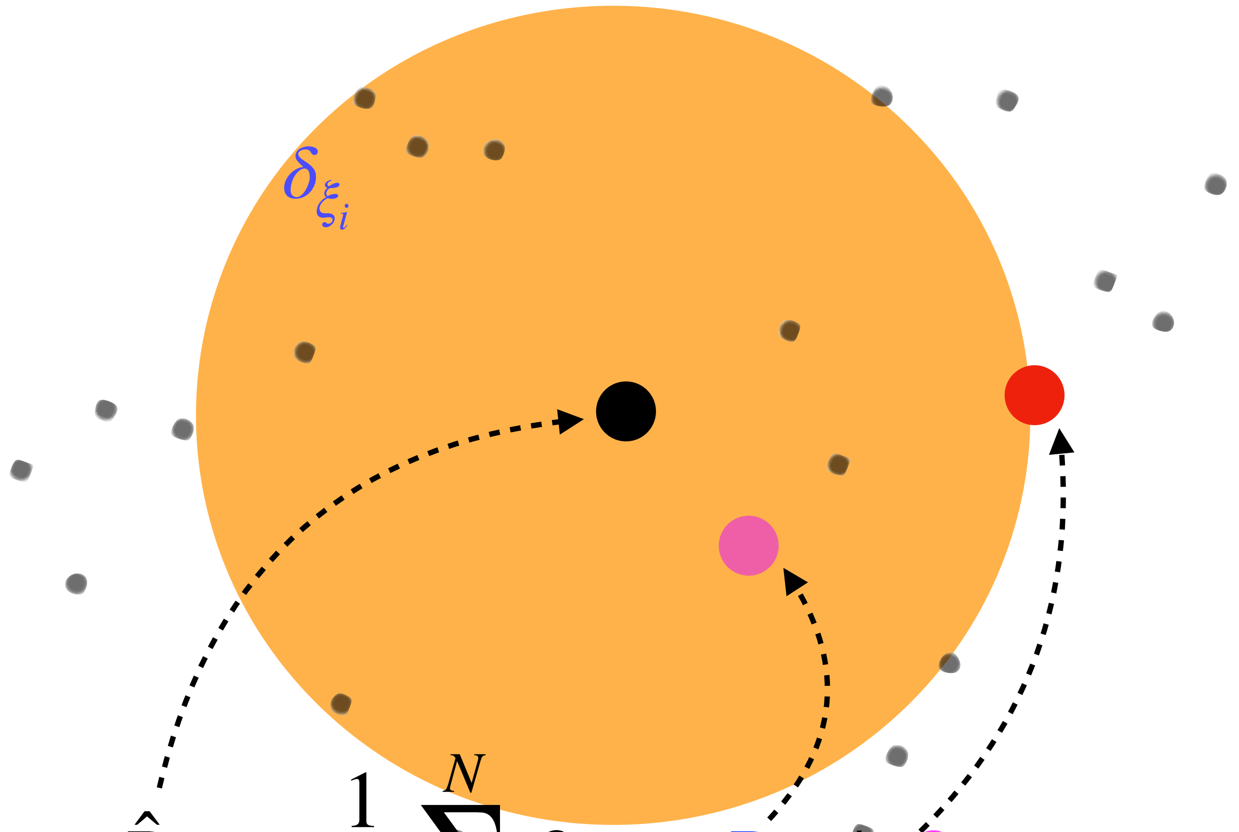

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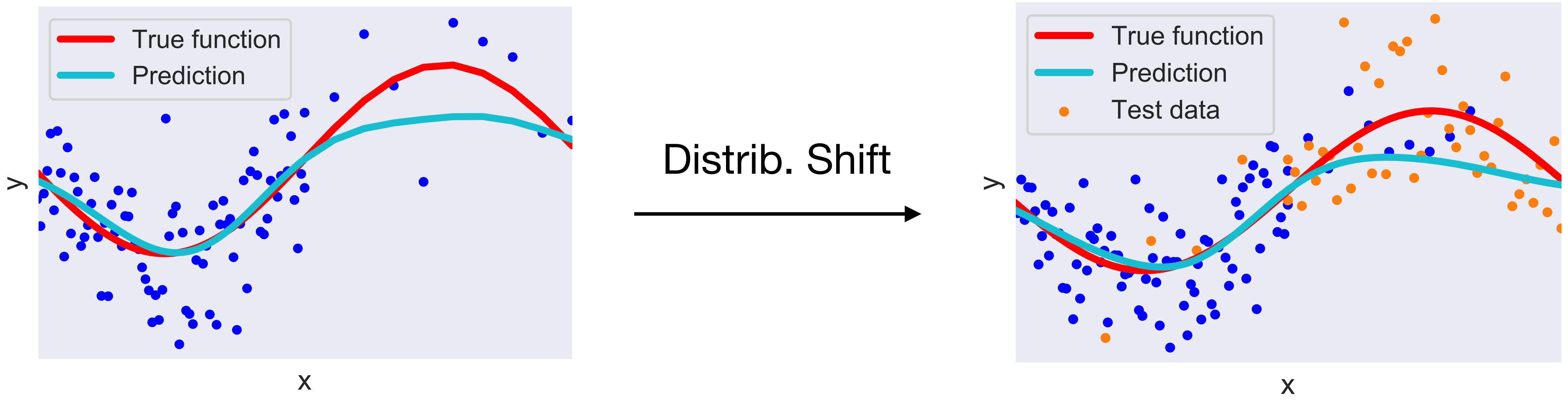

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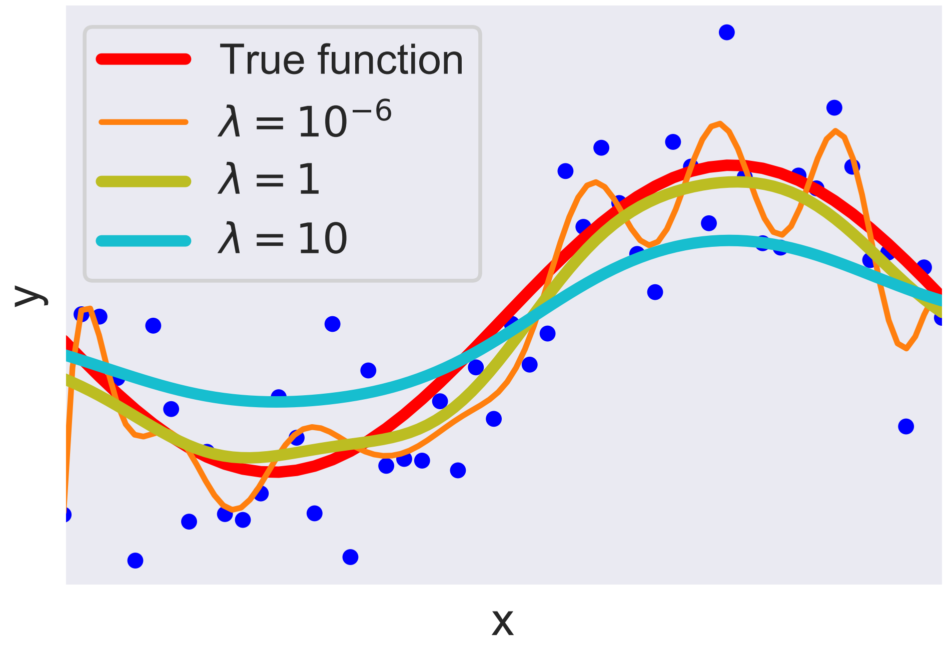

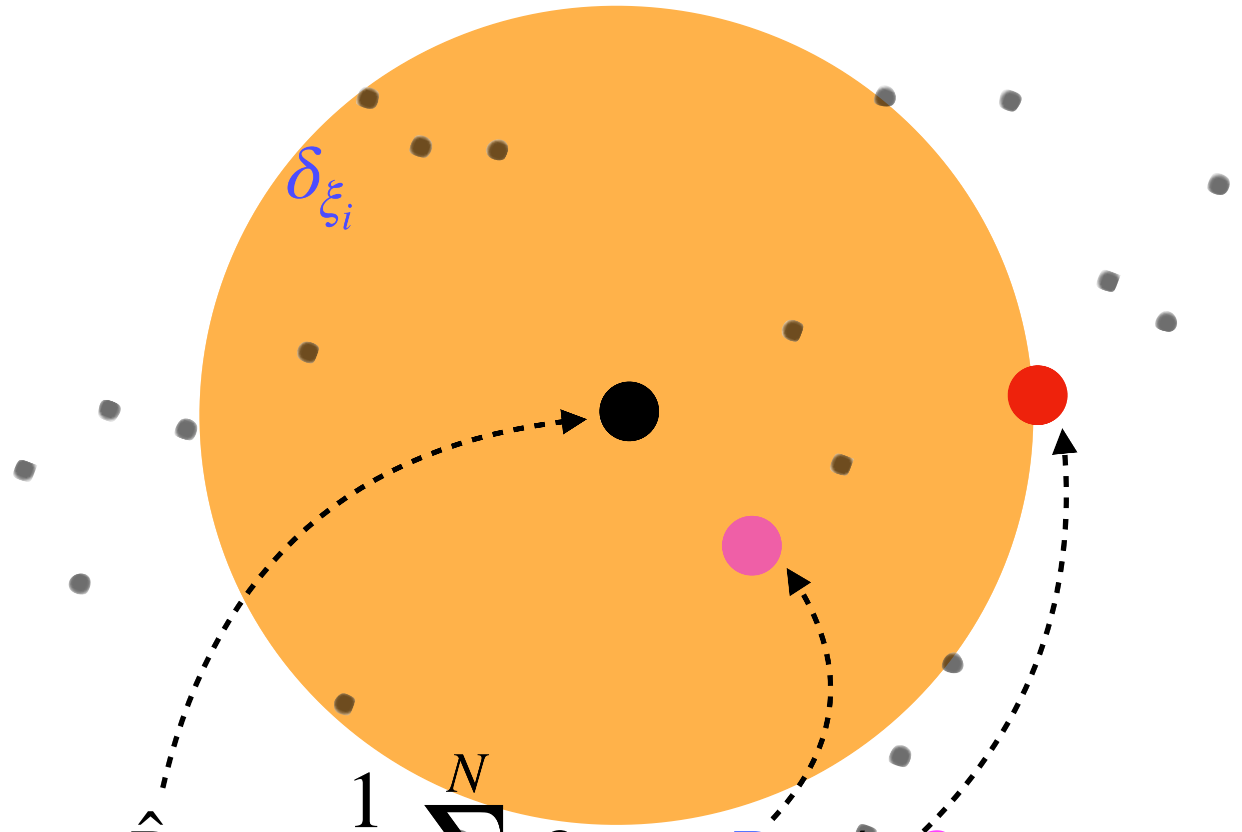

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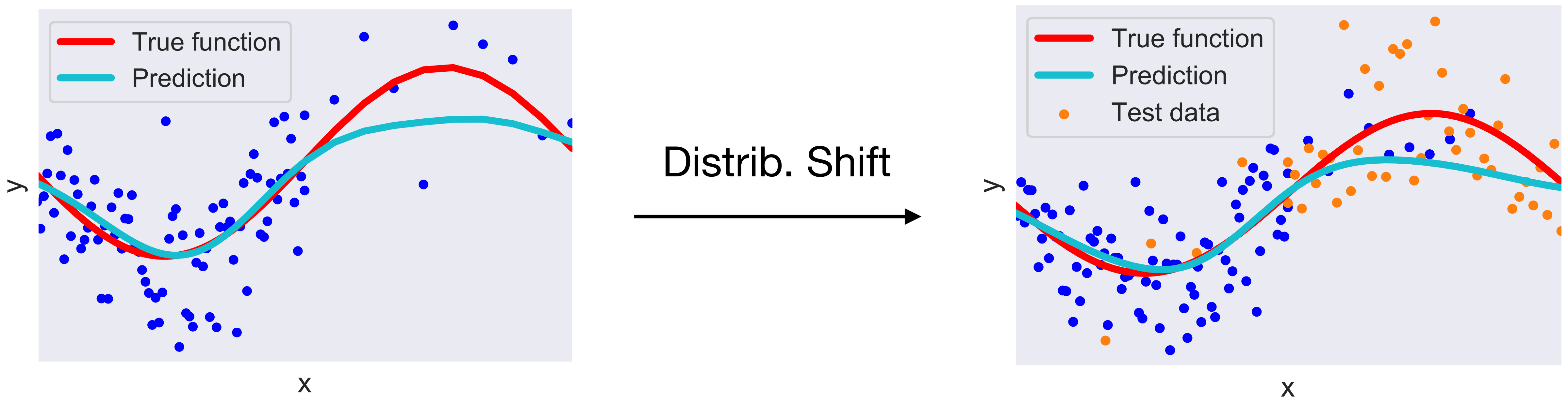

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Wasserstein Gradient flow [F. Otto et al.] e.g. Fokker-Planck equation as GF in W2

Figure credit: Heiner Kremer

Background: Wasserstein Geometry

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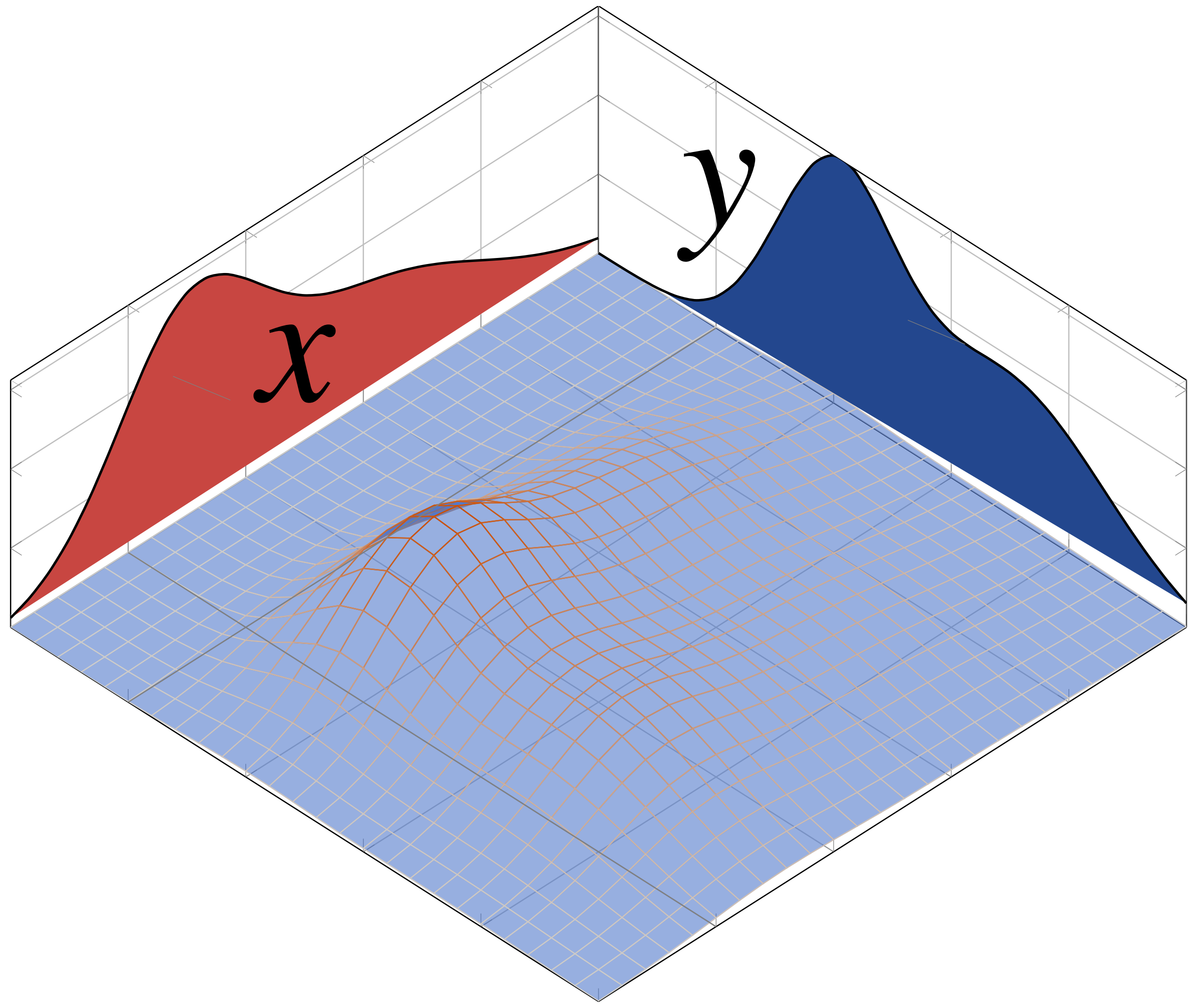

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$$W_p^p(P, Q) := \inf \left\{ \int |x-y|^p \, d\Pi(x,y) \,\middle|\, \pi_\#^{(1)}\Pi = P,\ \pi_\#^{(2)}\Pi = Q \right\}$$

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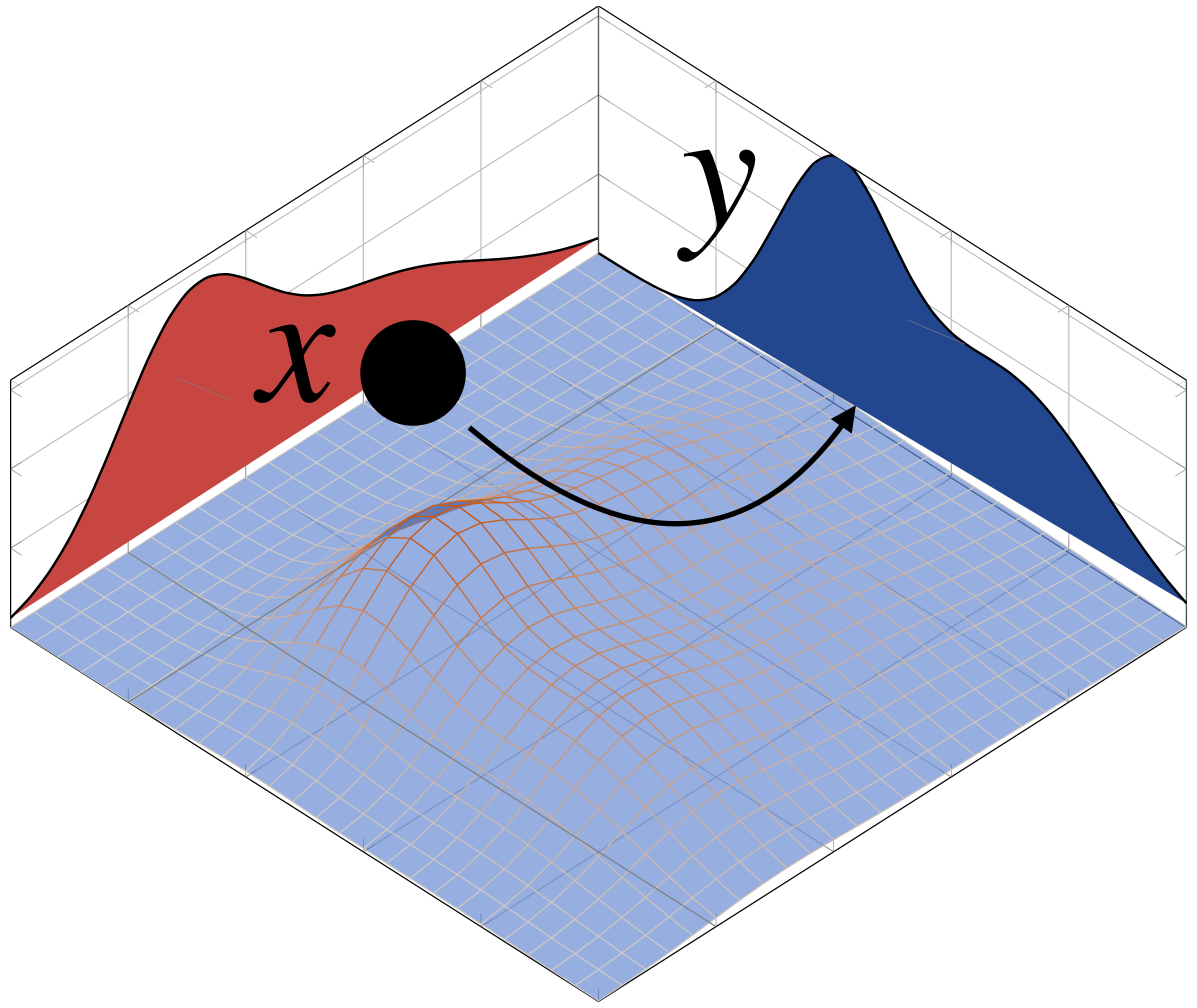

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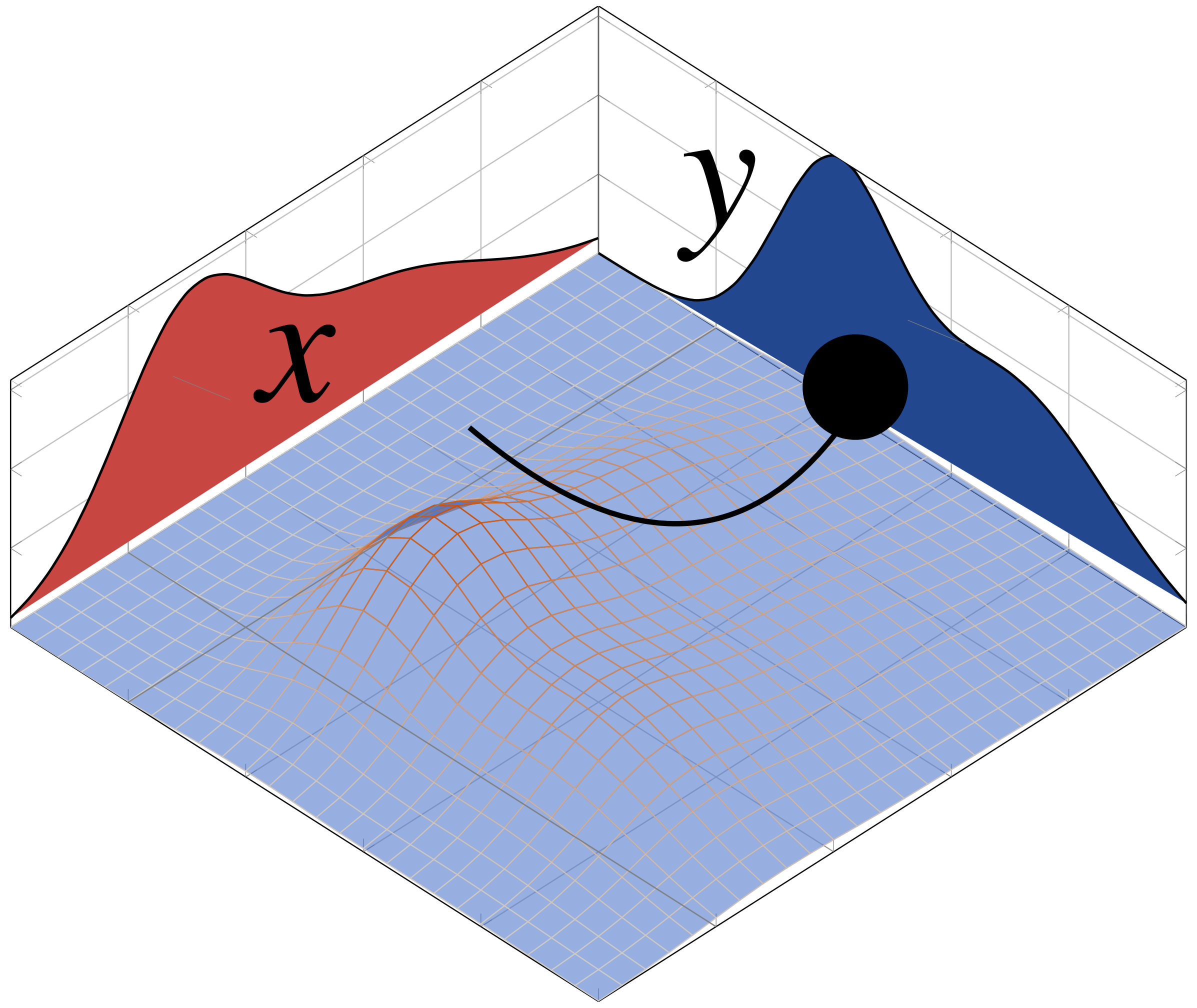

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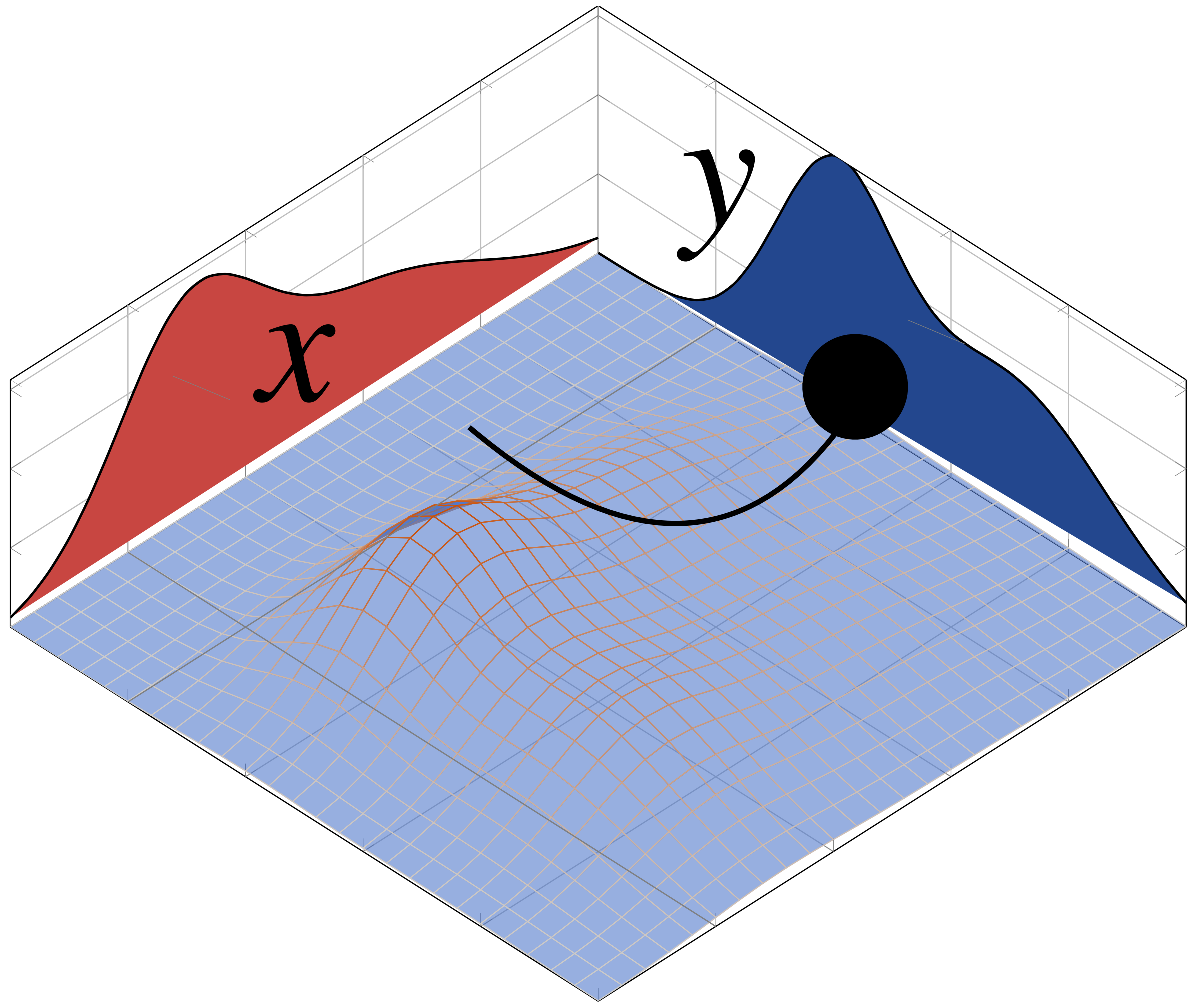

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(**Dual Kantorovich problem**)

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

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

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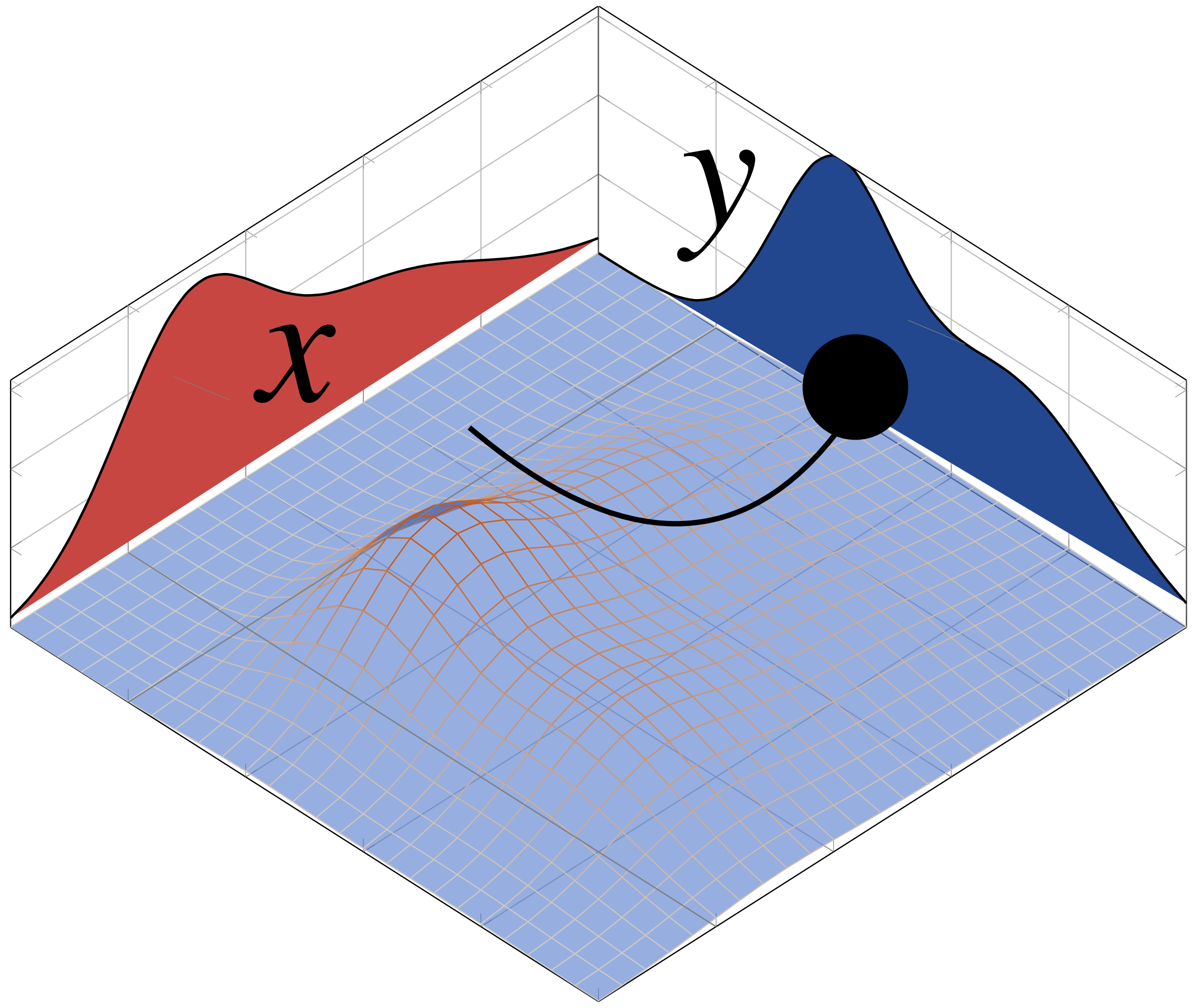

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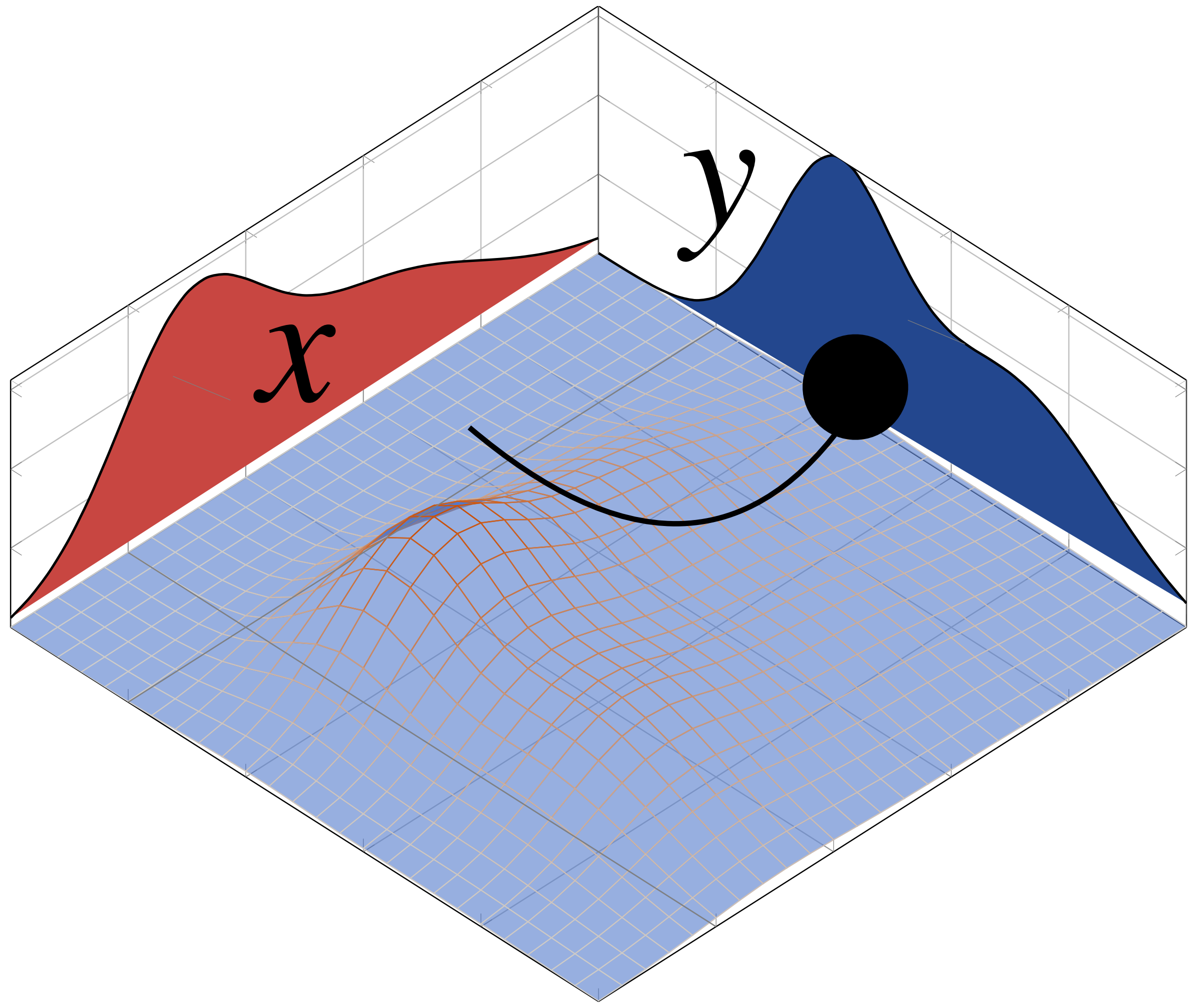

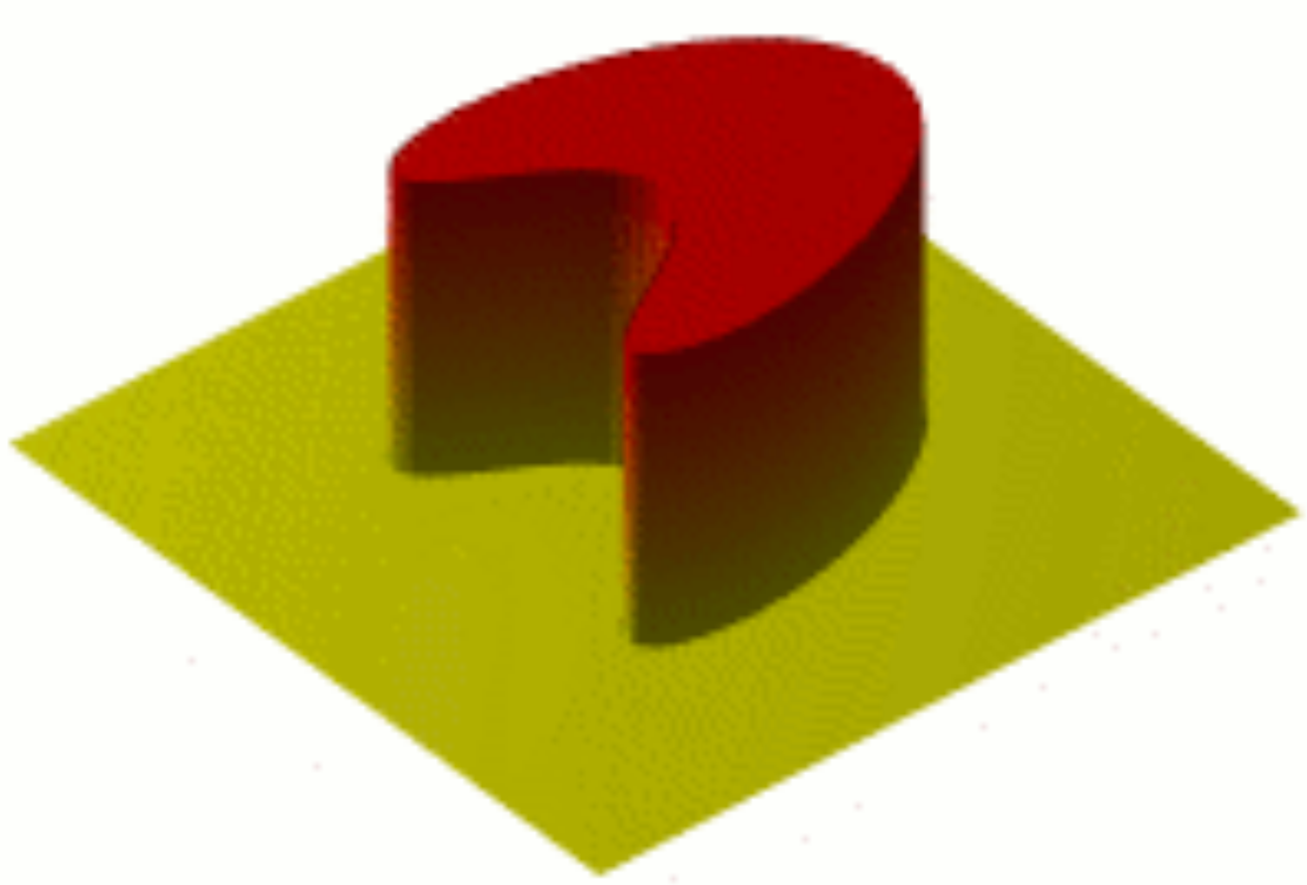

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Definition. Kernel **Maximum-Mean Discrepancy** (MMD) associated with (PSD) kernel k (e.g., $k(x,x') := e^{-|x-x'|^2/\sigma}$)

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

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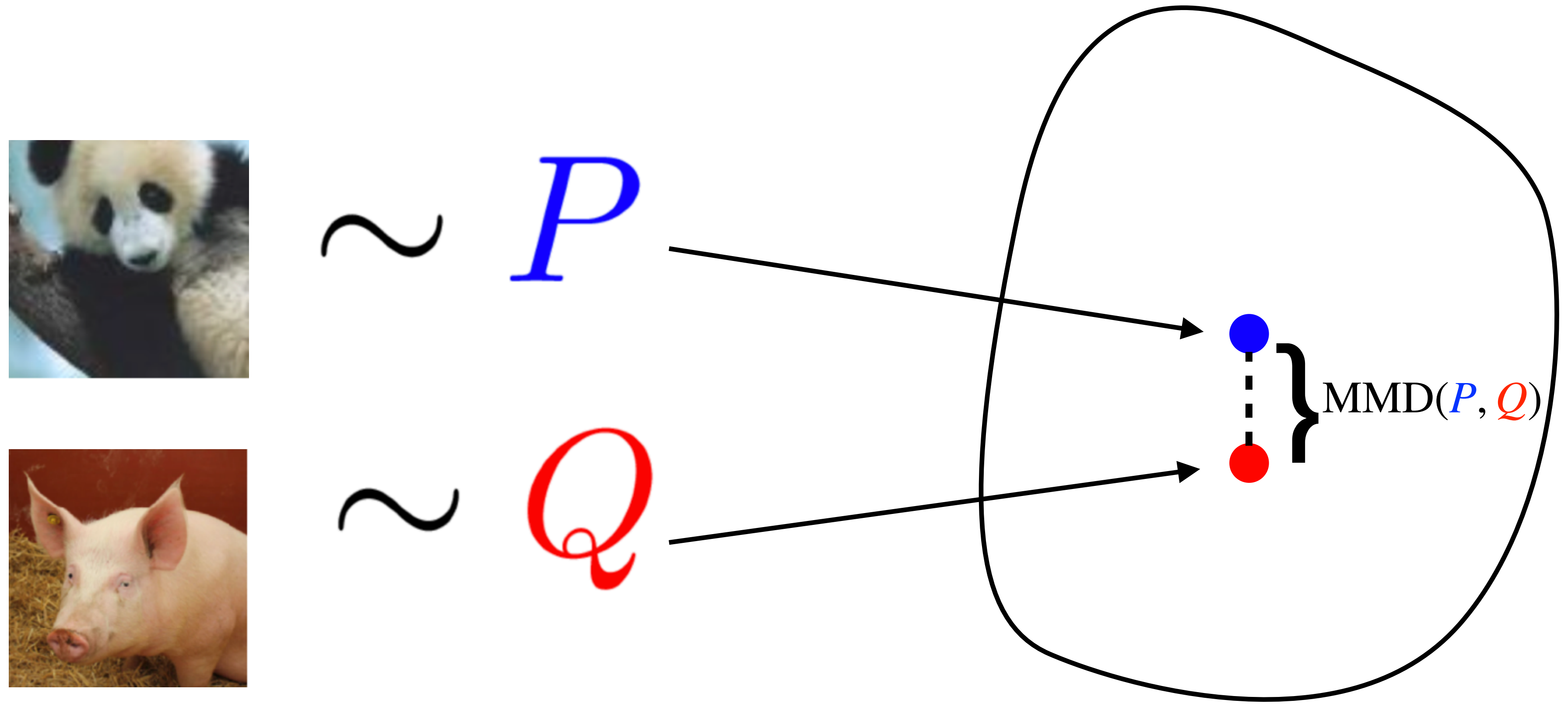

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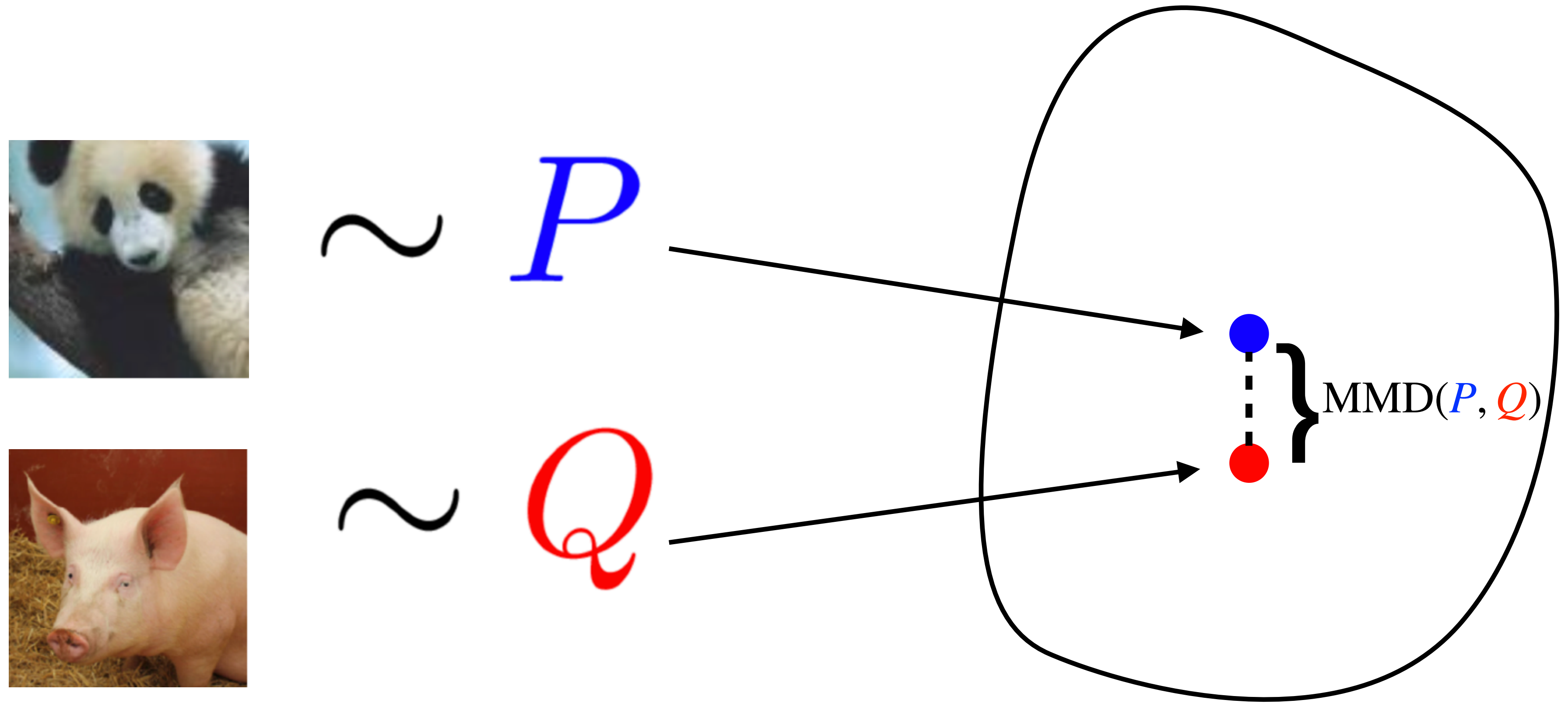
Dual formulation as an integral probability metric.

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

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



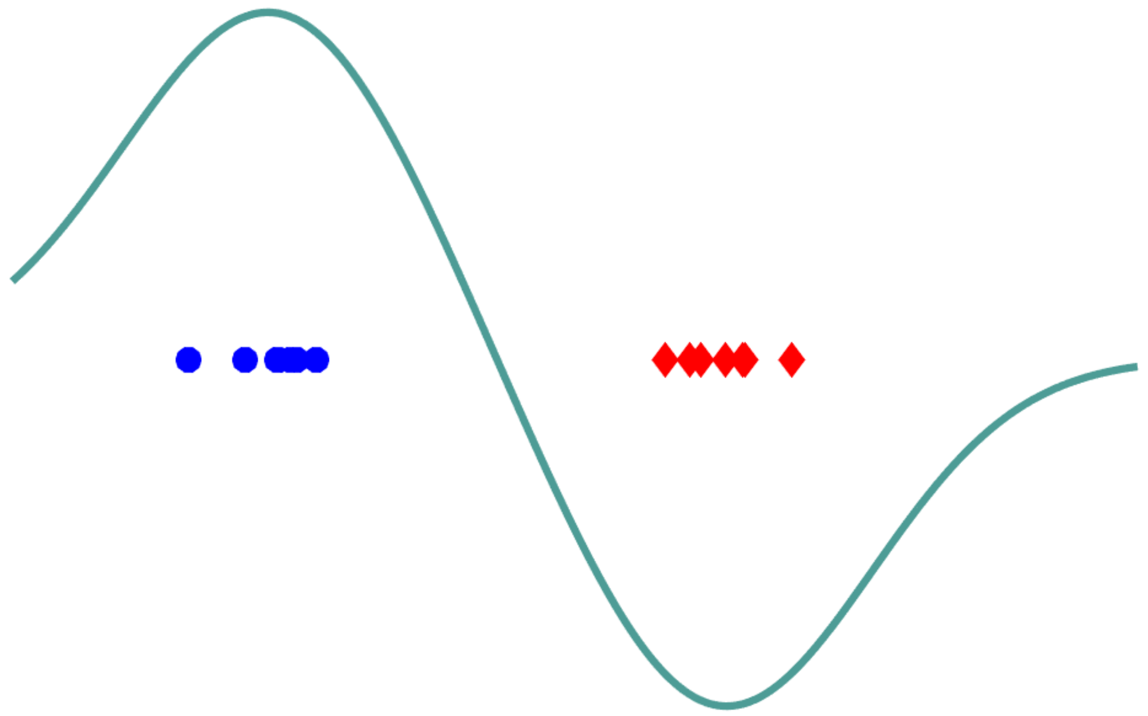


Figure credit: W. Jitkrittum, J. Zhu

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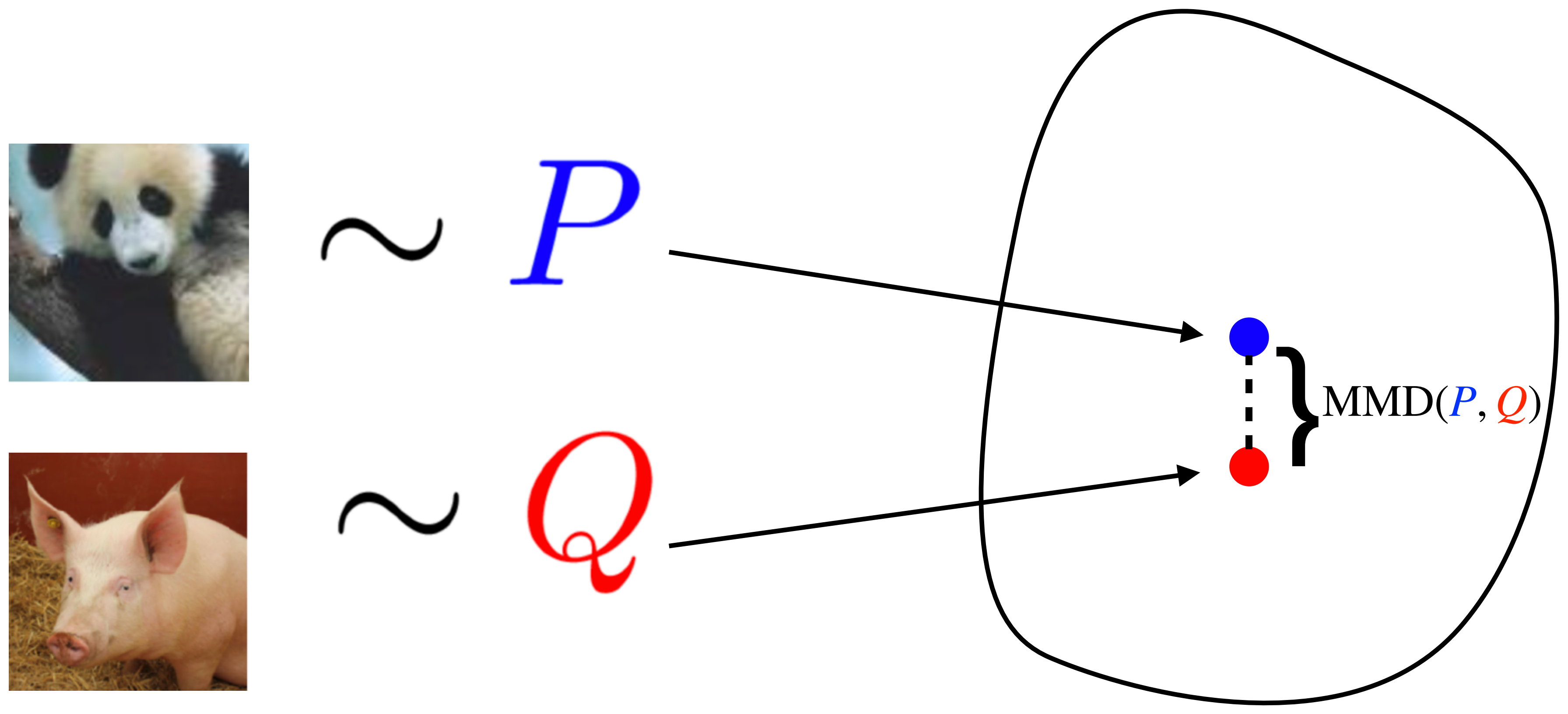
Example. Approx. nonlinear functions



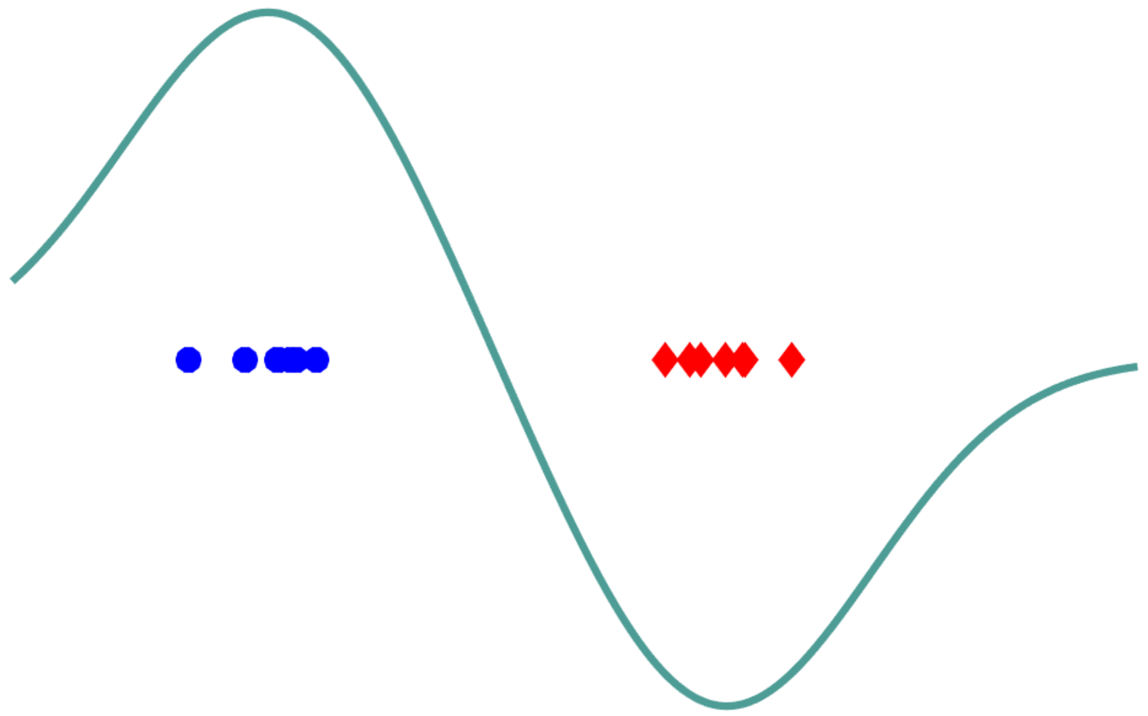


Figure credit: W. Jitkrittum, J. Zhu

Background: "Kernel Geometry"

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

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

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

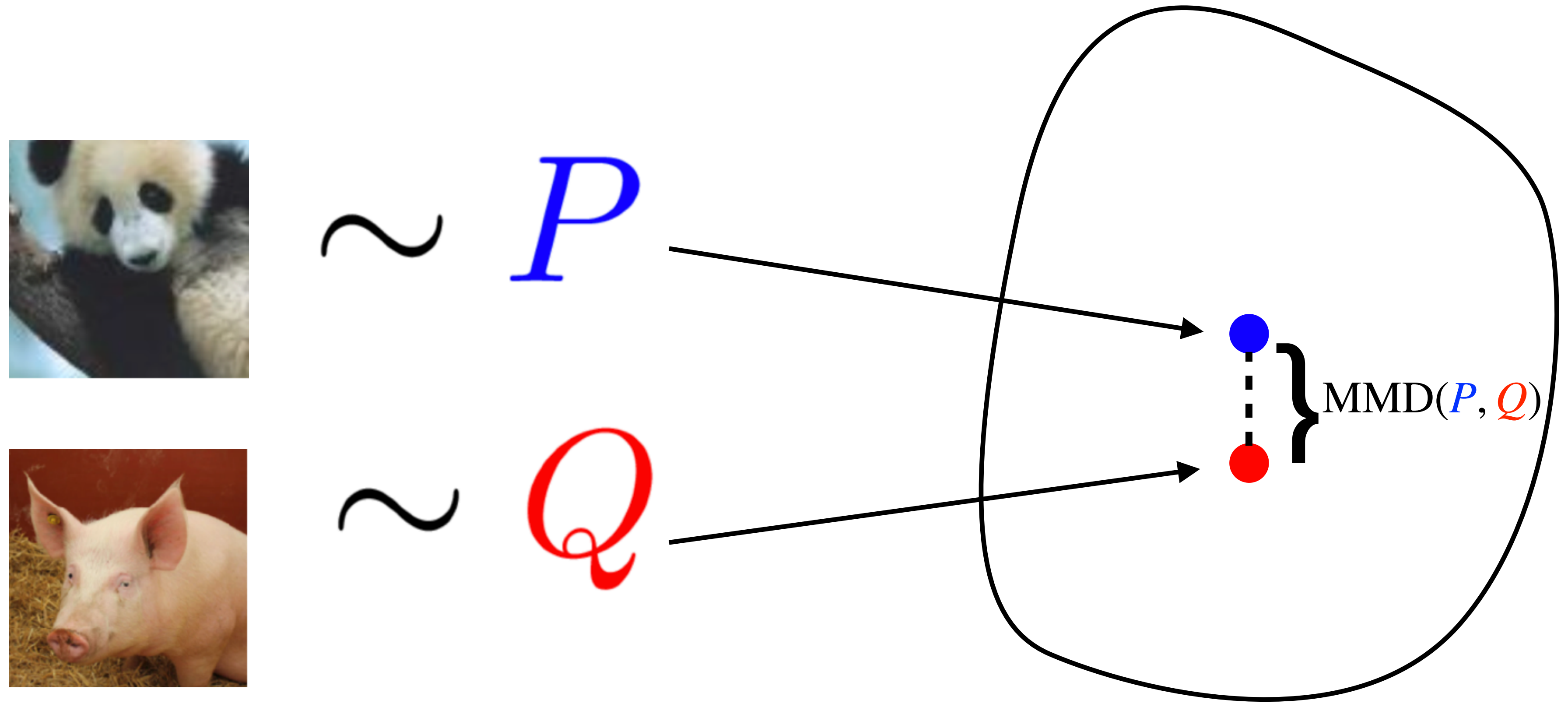
Dual formulation as an integral probability metric.

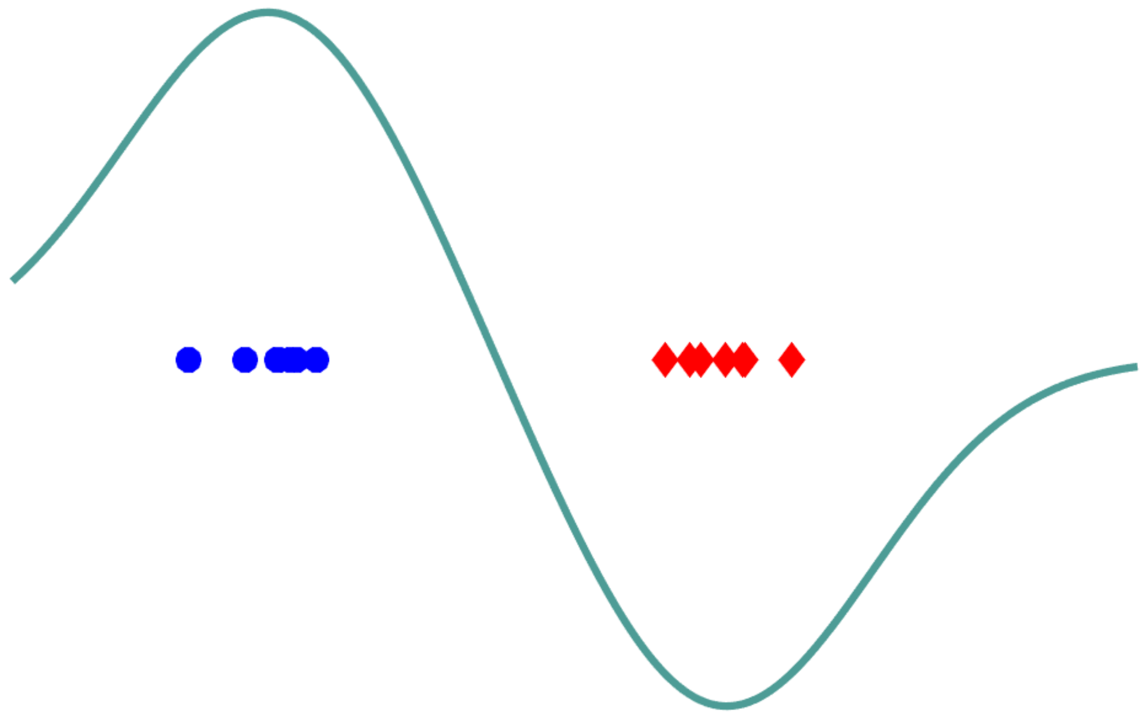
$$\mathrm{MMD}(P, Q) = \sup_{\|f\|_{\mathcal{H}} \le 1} \int f\, d(P - Q)$$

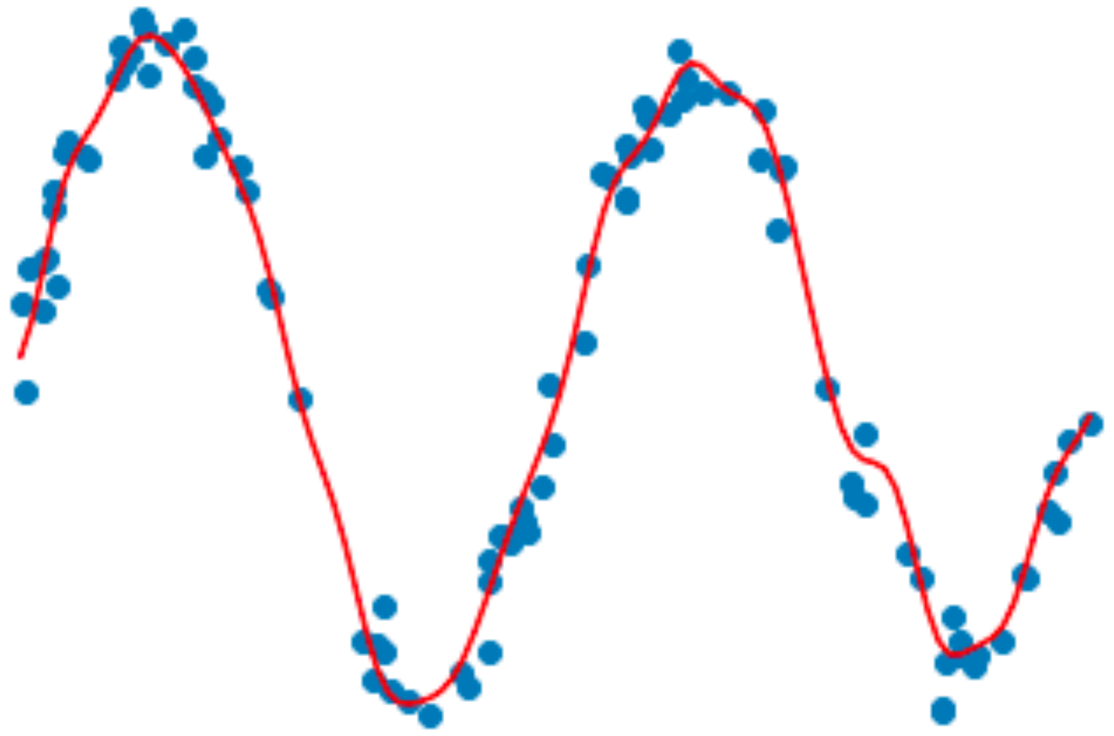
$\mathcal{H}$ is the **reproducing kernel Hilbert space** $\mathcal{H}$ (RKHS), which satisfies $f(x) = \langle f, \phi(x) \rangle_{\mathcal{H}}, \forall f \in \mathcal{H}, x \in \mathcal{X}$, $\phi(x) := k(x, \cdot\,)$ is the canonical feature of $\mathcal{H}$.

Example. Approx. nonlinear functions

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







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Previous work: Kernel DRO

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Primal DRO (not solvable as it is)

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

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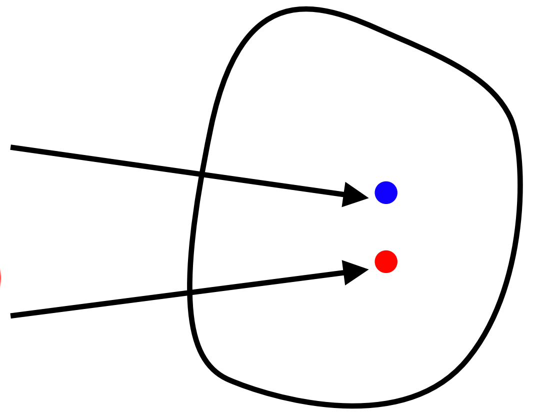

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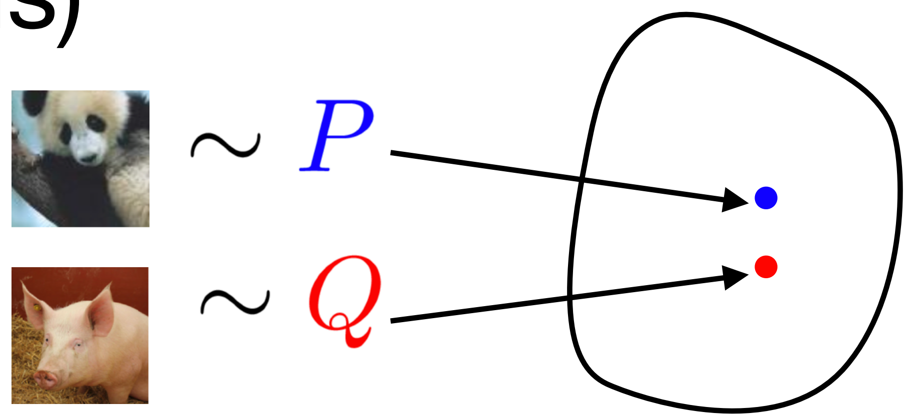

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DRO problem is equivalent to the dual kernel machine learning problem, i.e., (DRO)=(K).

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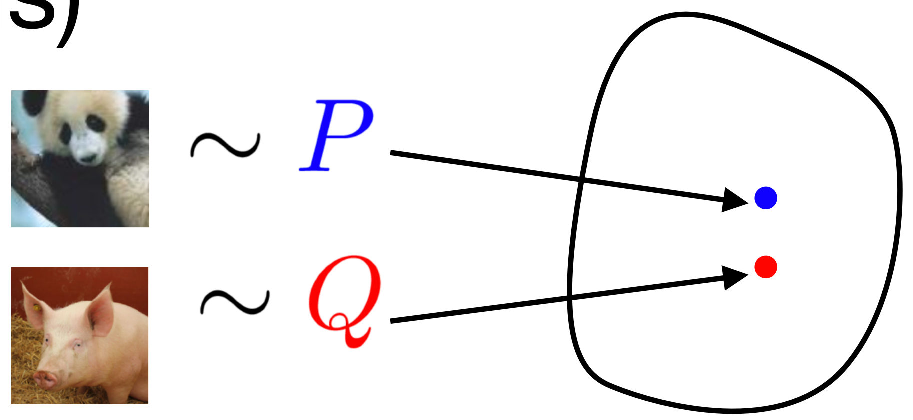

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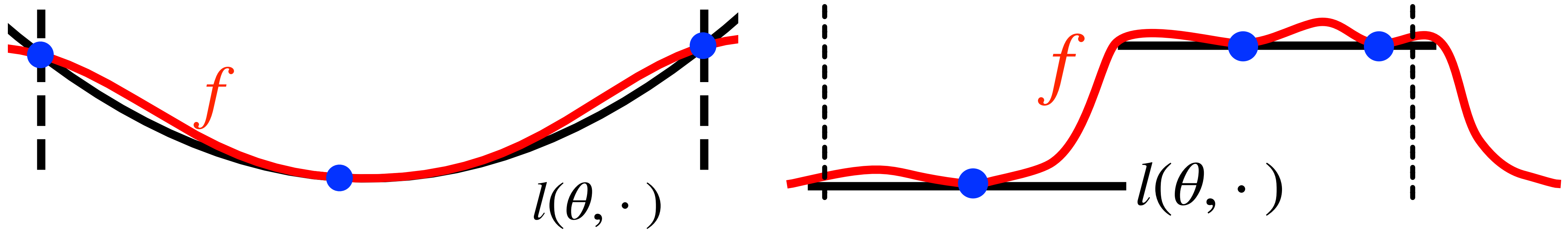

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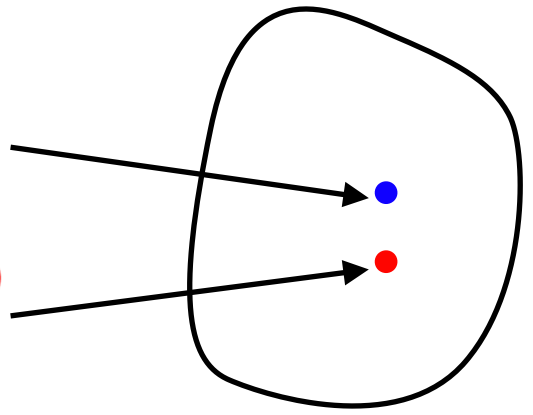

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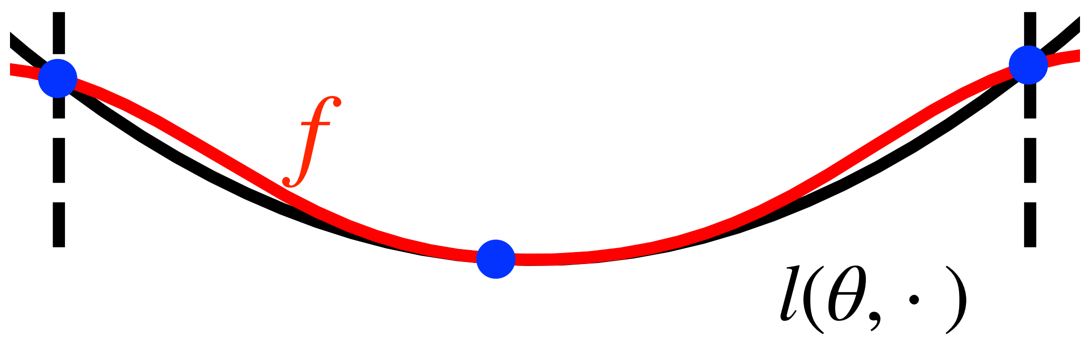
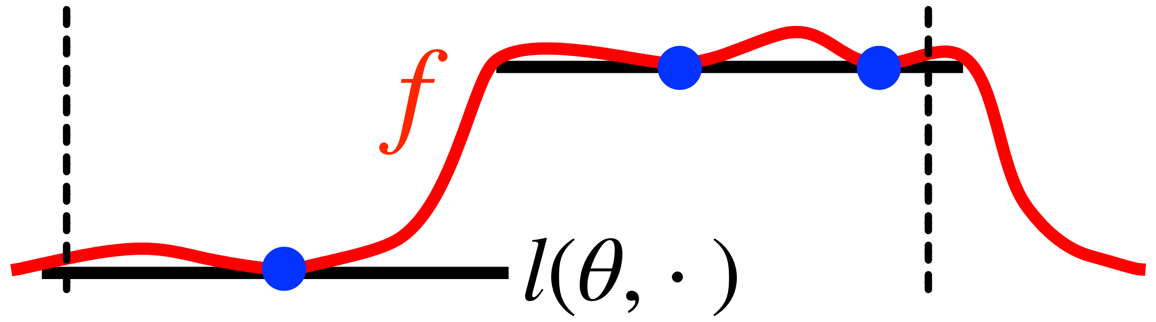
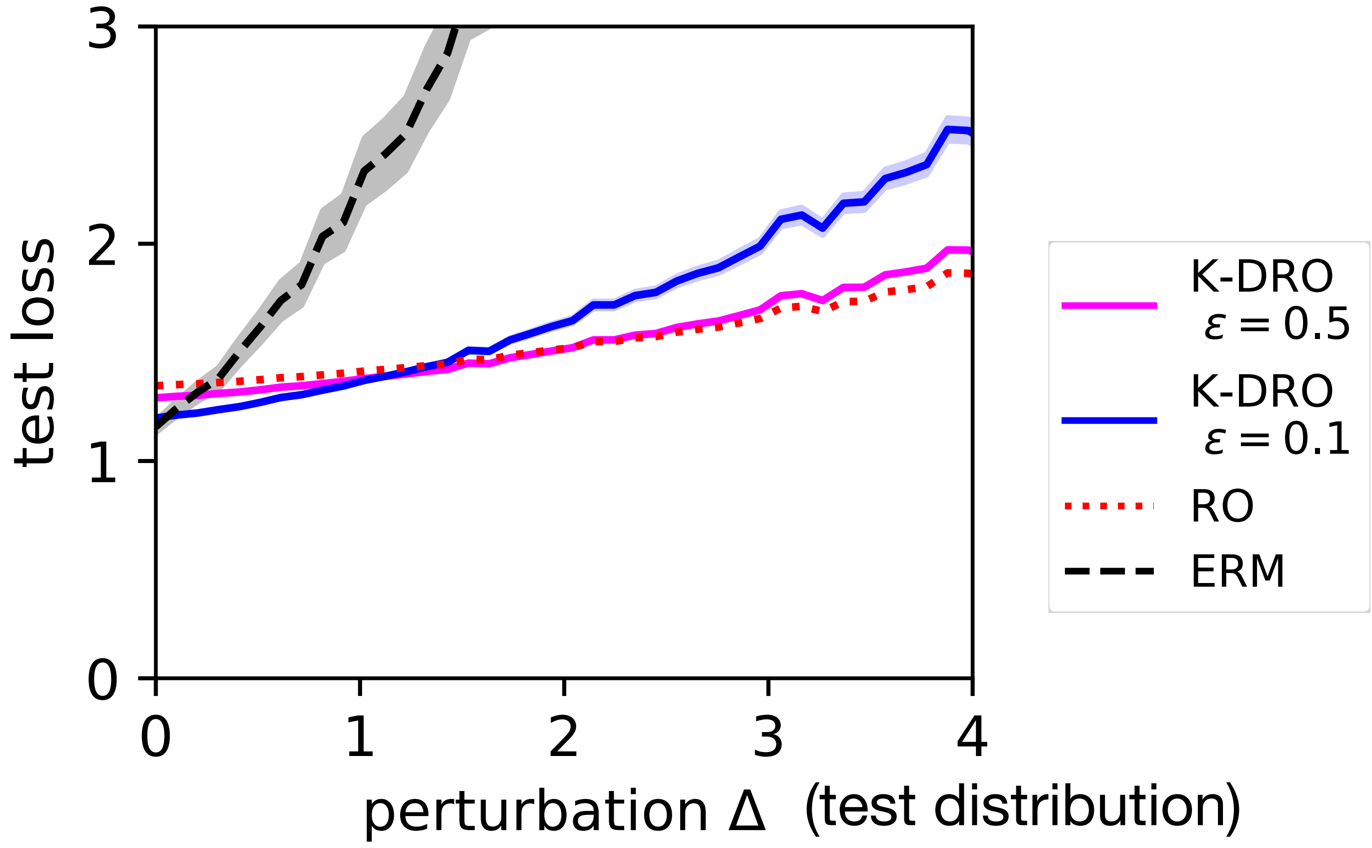




Example. Robust least squares
[El Ghaoui Lebret '97]

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

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



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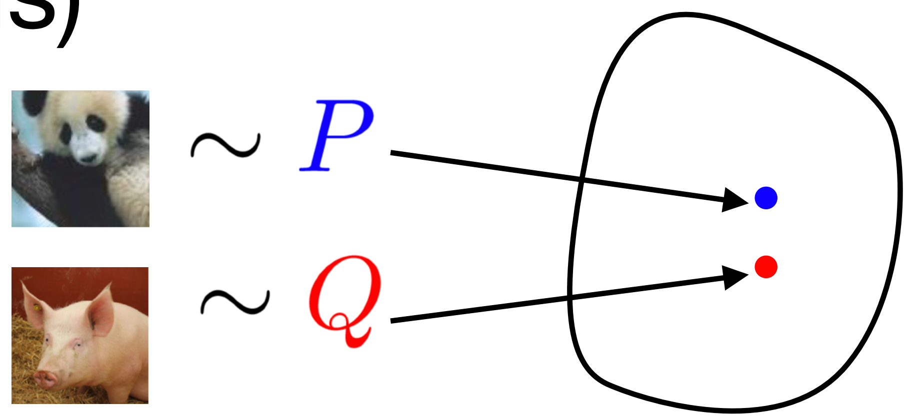

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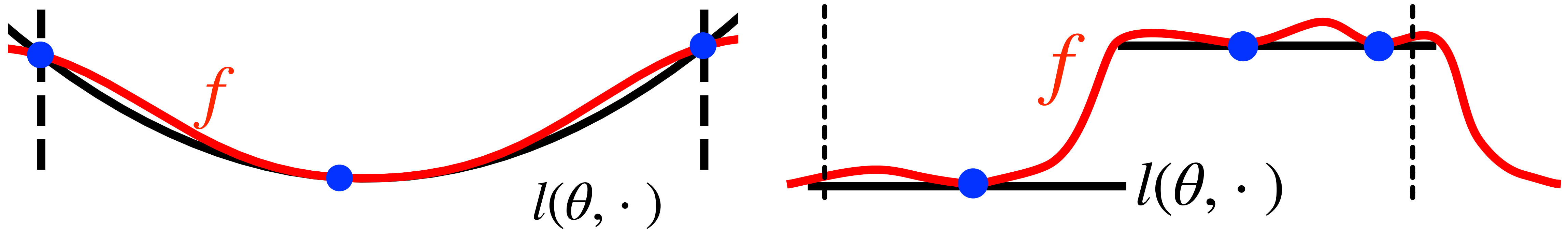

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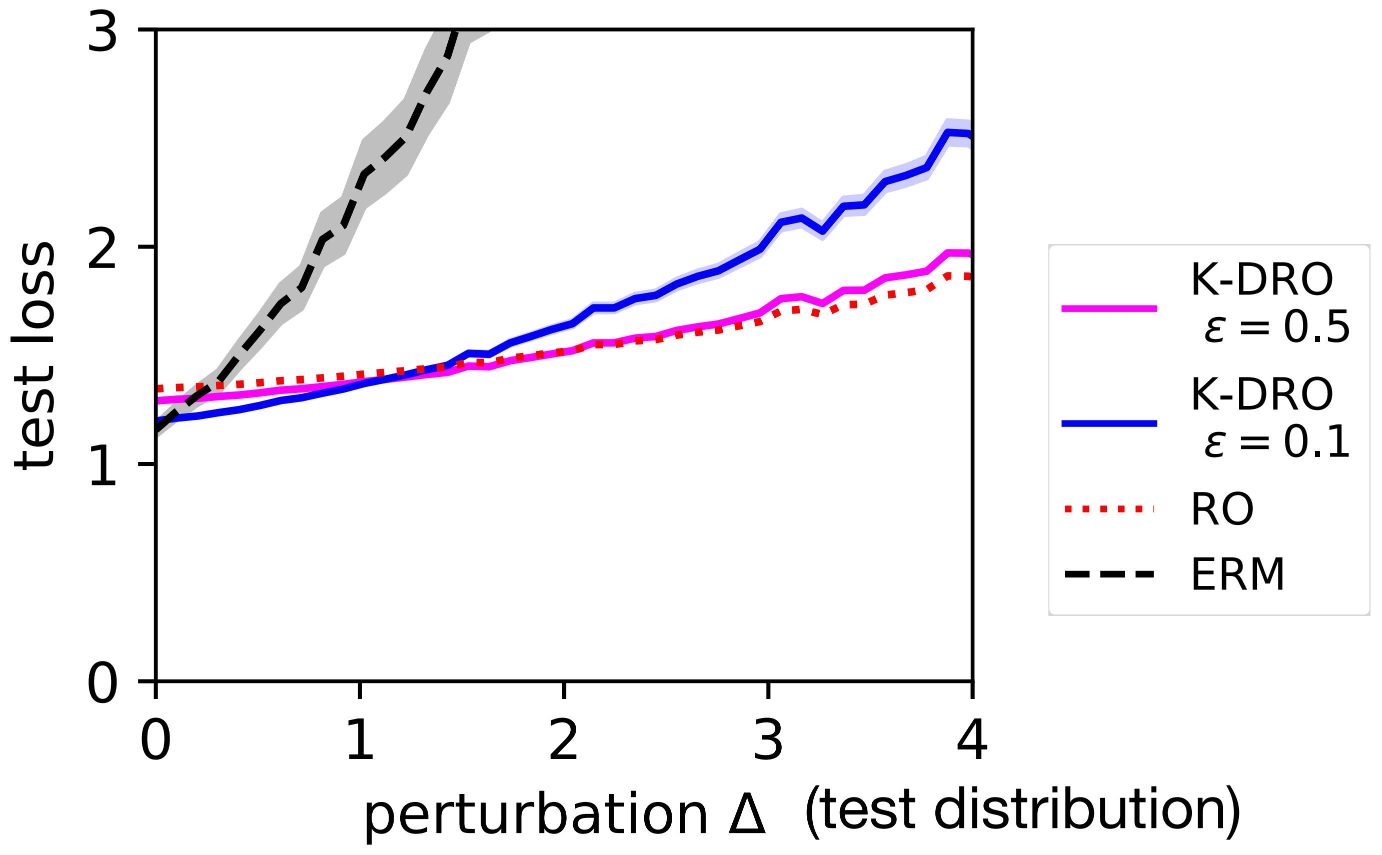
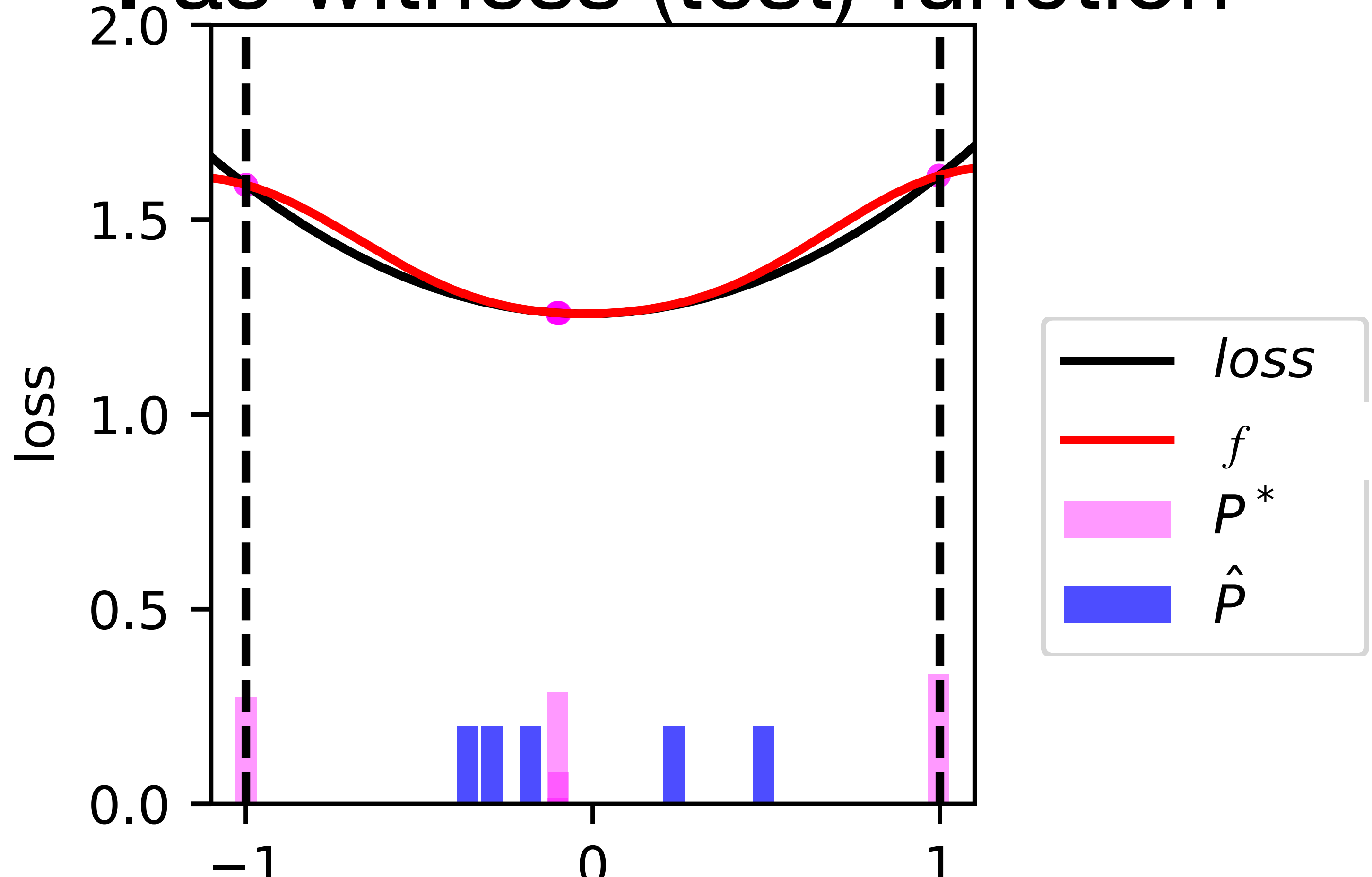


Robustifying with DRO

f as witness (test) function



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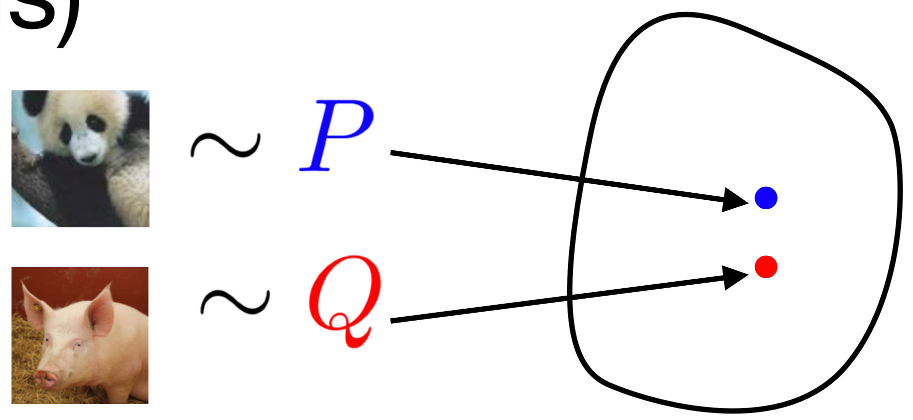

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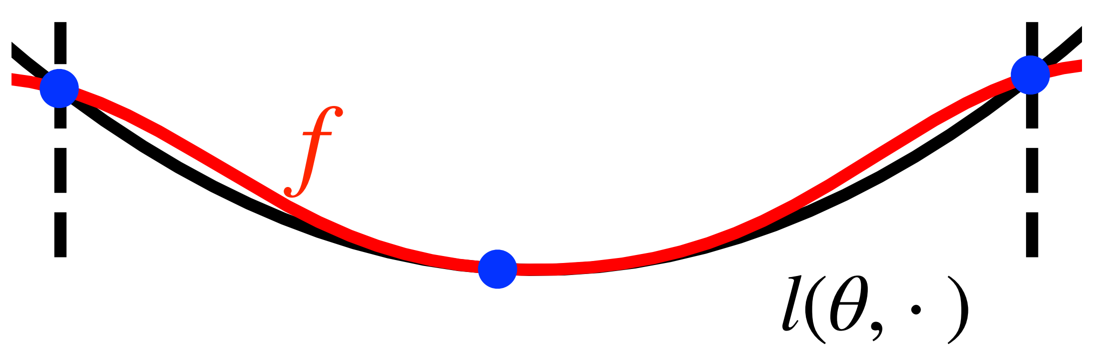

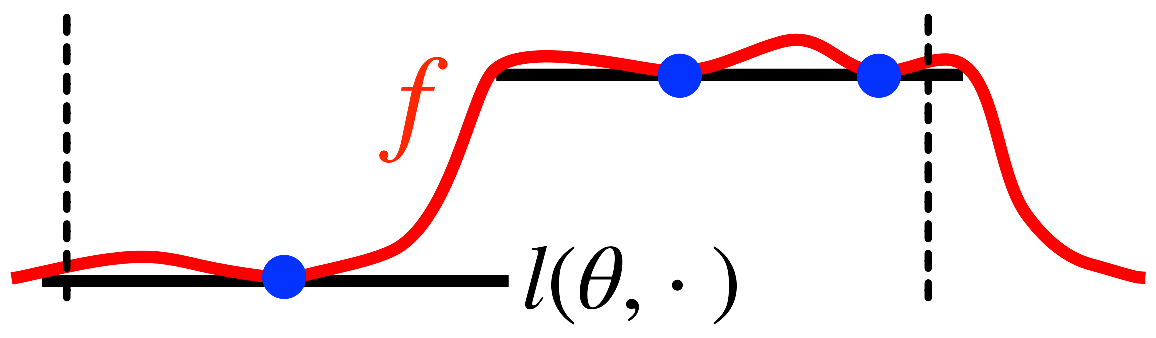

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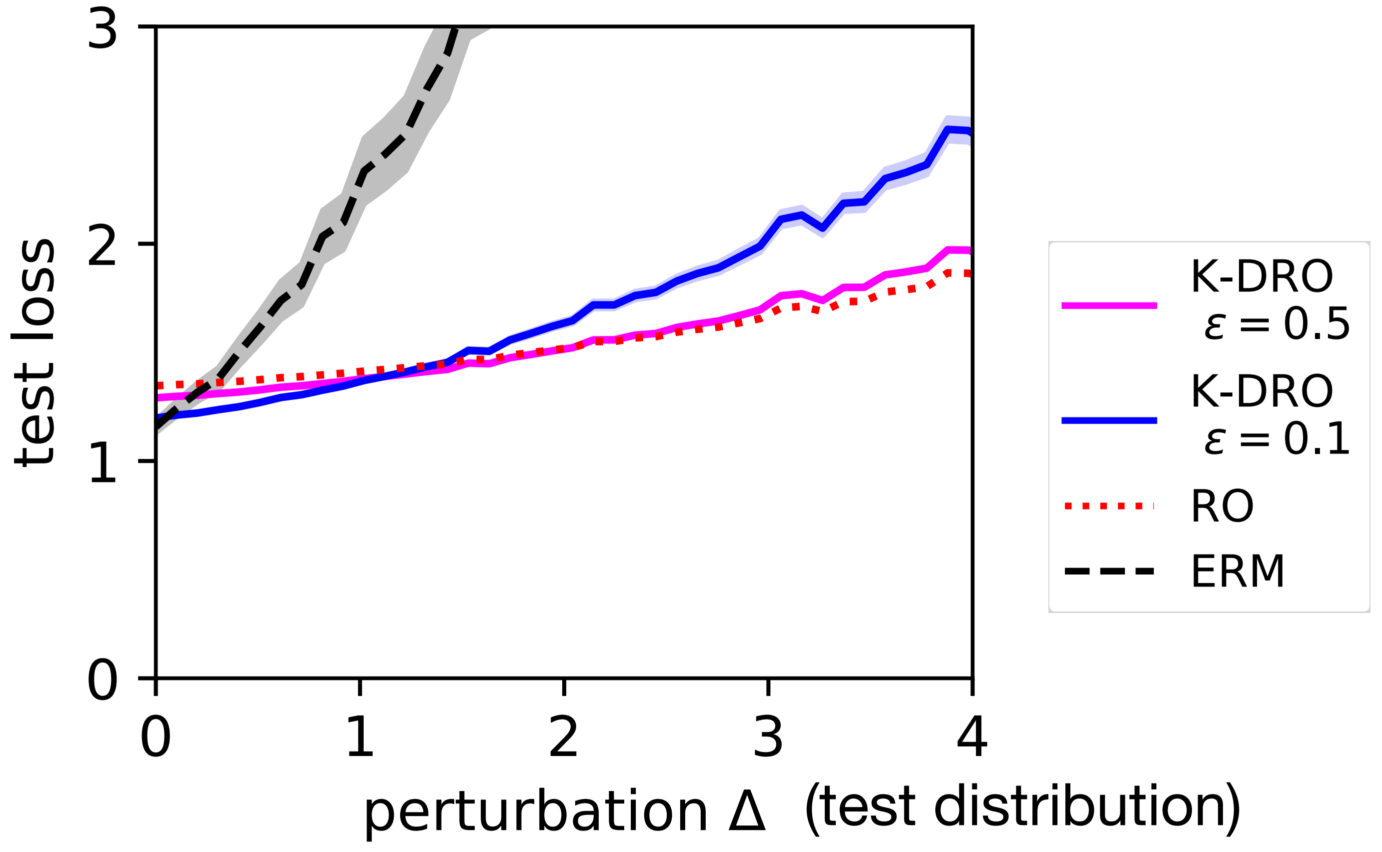

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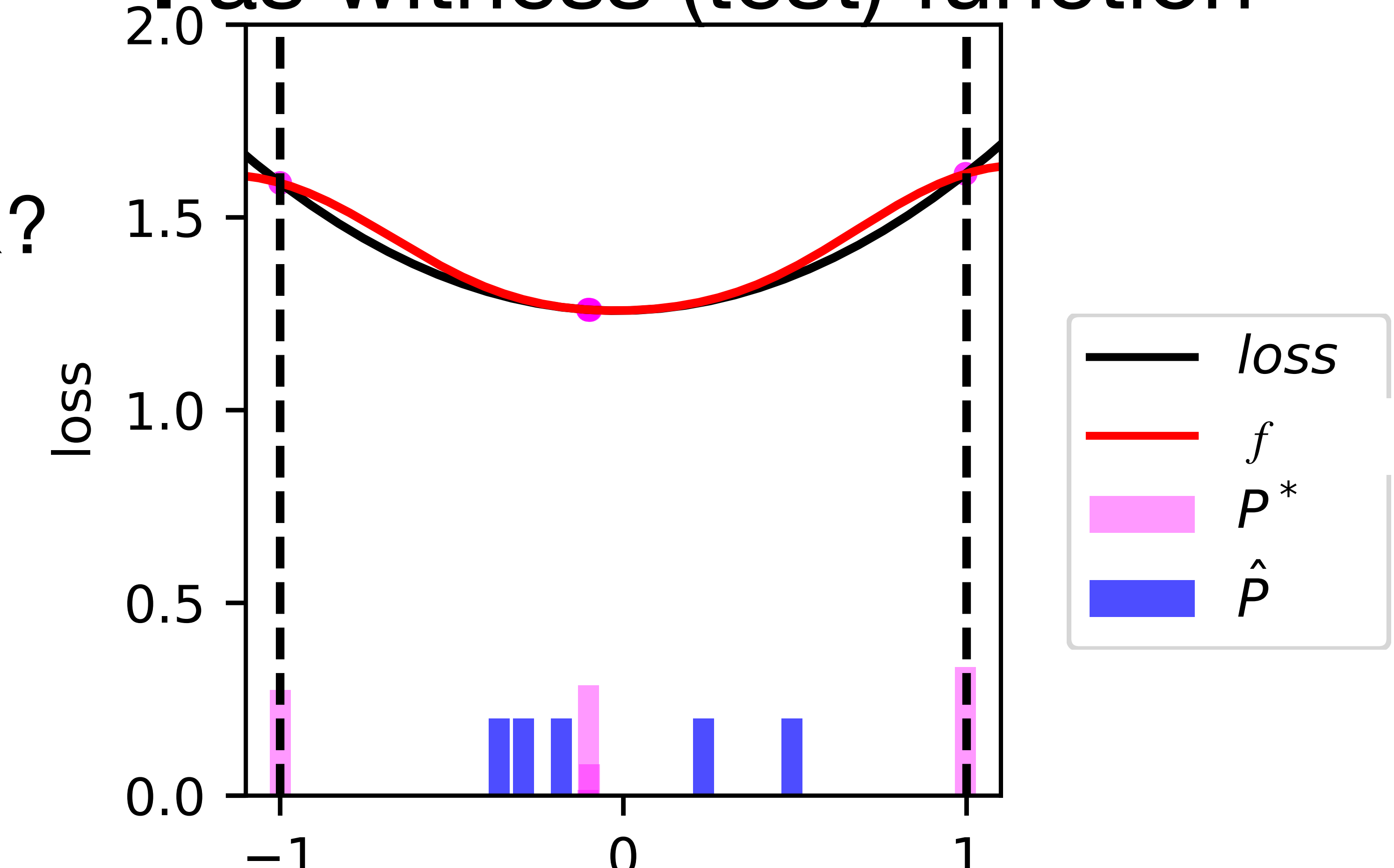

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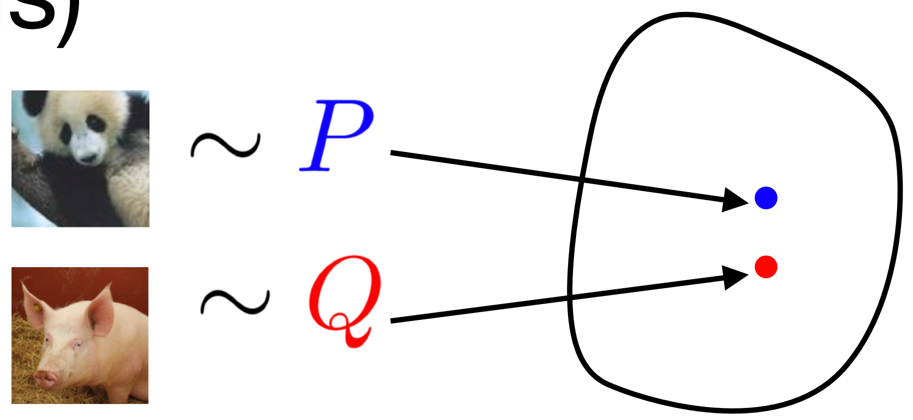

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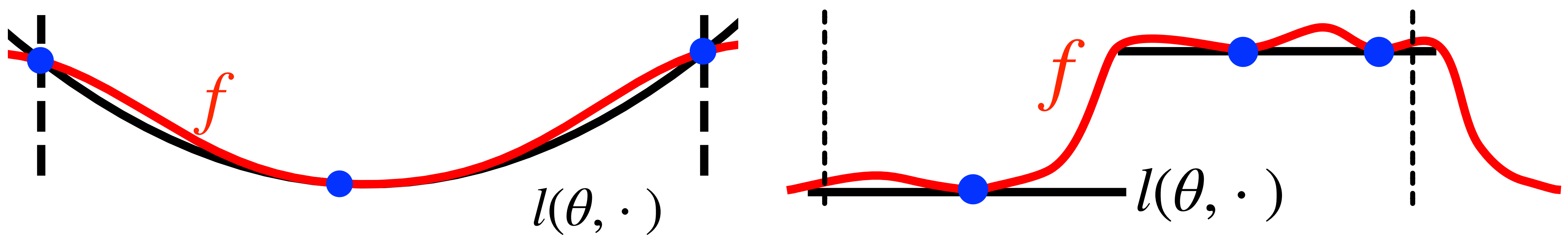

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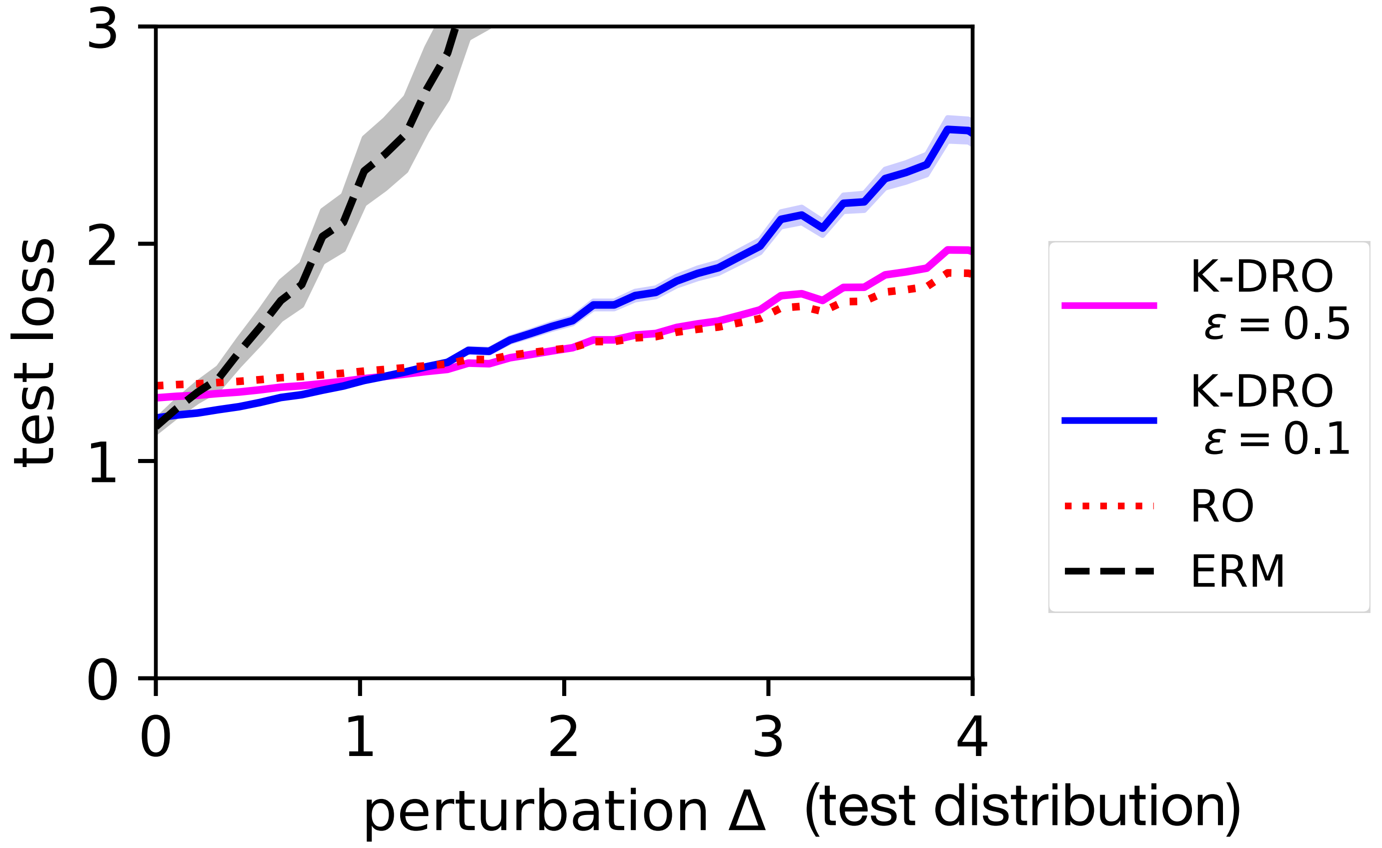

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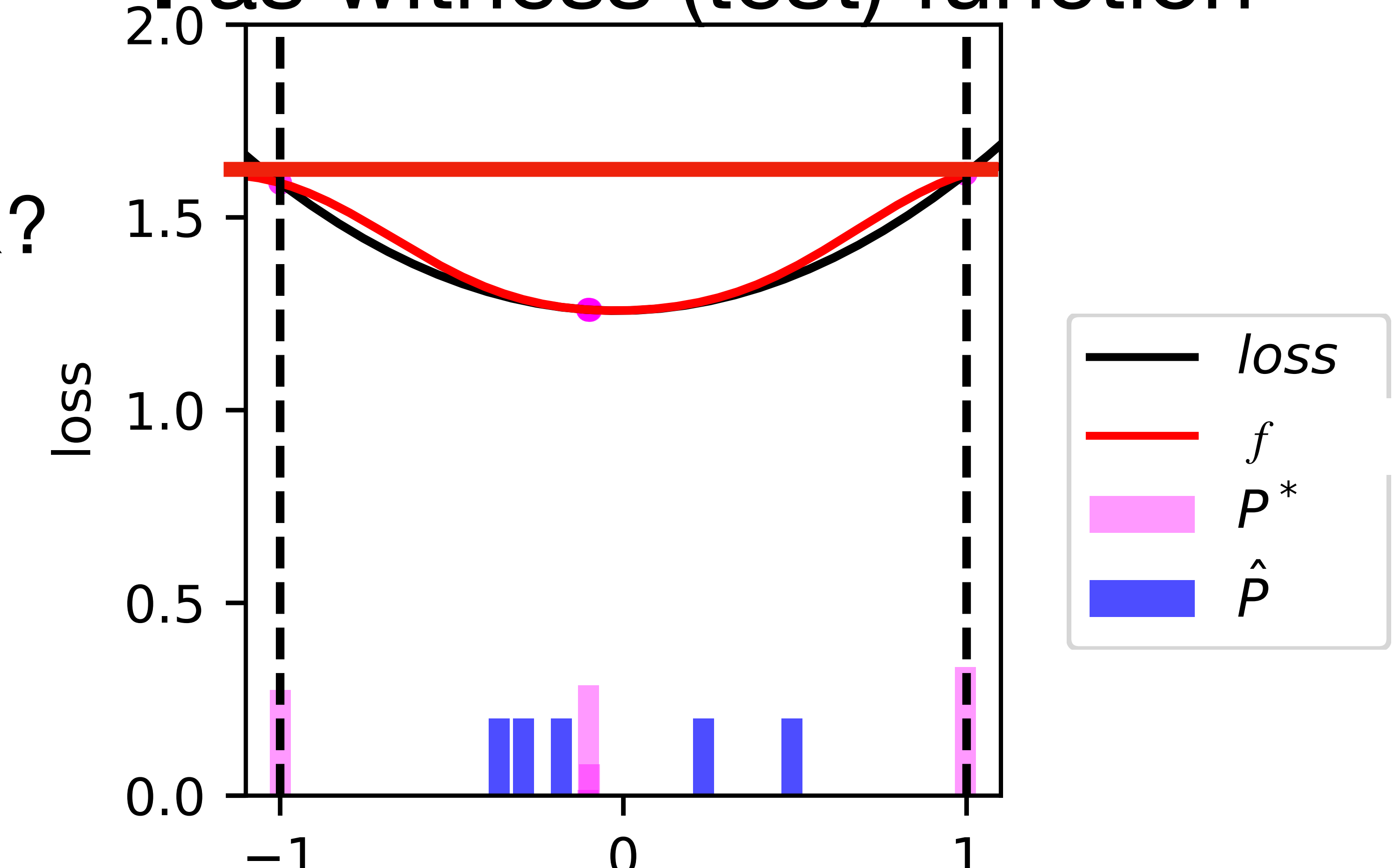

Duality perspective

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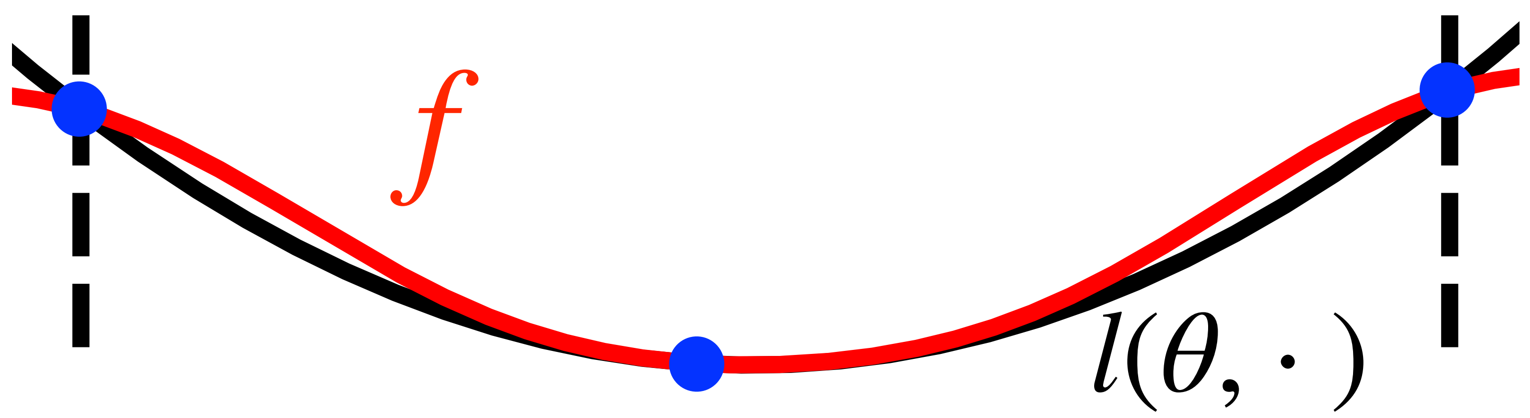

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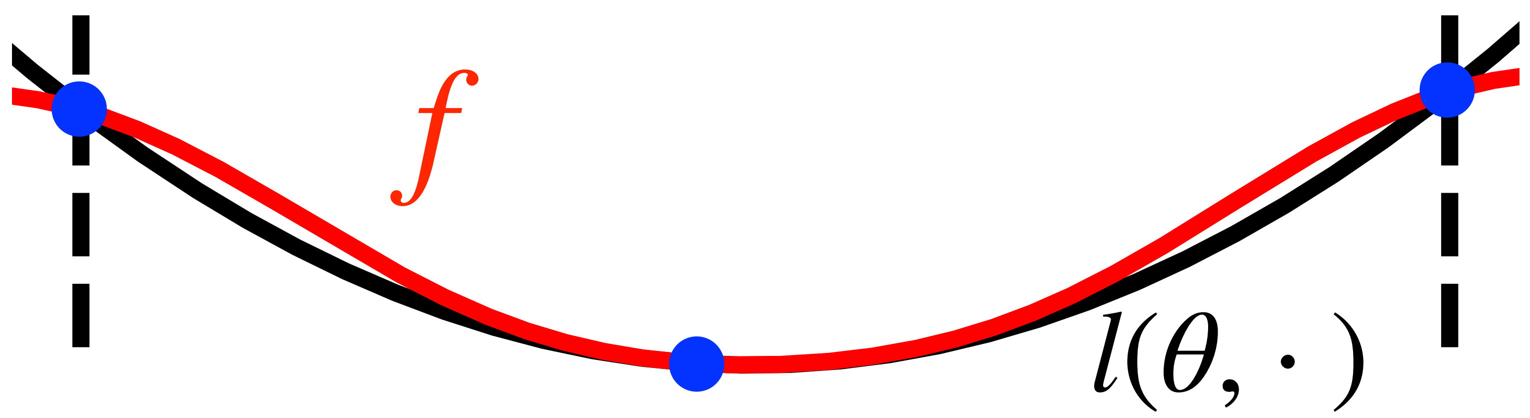

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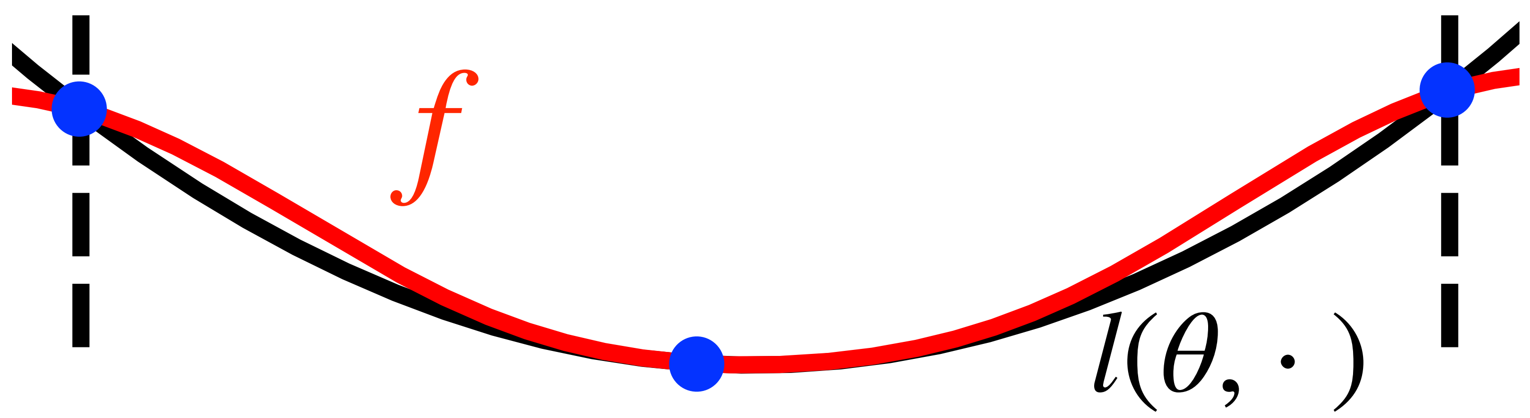

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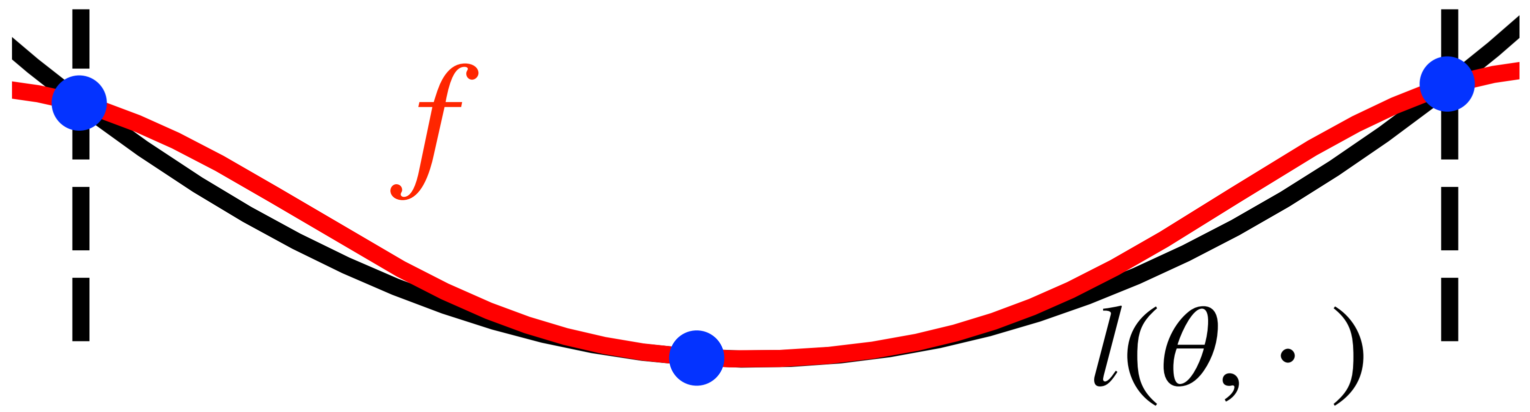

Nonlinear kernel approx. as robust surrogate losses (<u>flatten the curve</u>)

Duality of
Gradient Flow Force-Balance

From static DRO to JKO scheme for gradient flows

DRO's Wasserstein measure optimization is not new.

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

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

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

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

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

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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**)

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

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

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

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

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

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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

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

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

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

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