Robust Optimization and Machine Learning under Distribution Shift

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Leibniz MMS Summer School, Dagstuhl
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Distributional Robustness

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What is robustness?

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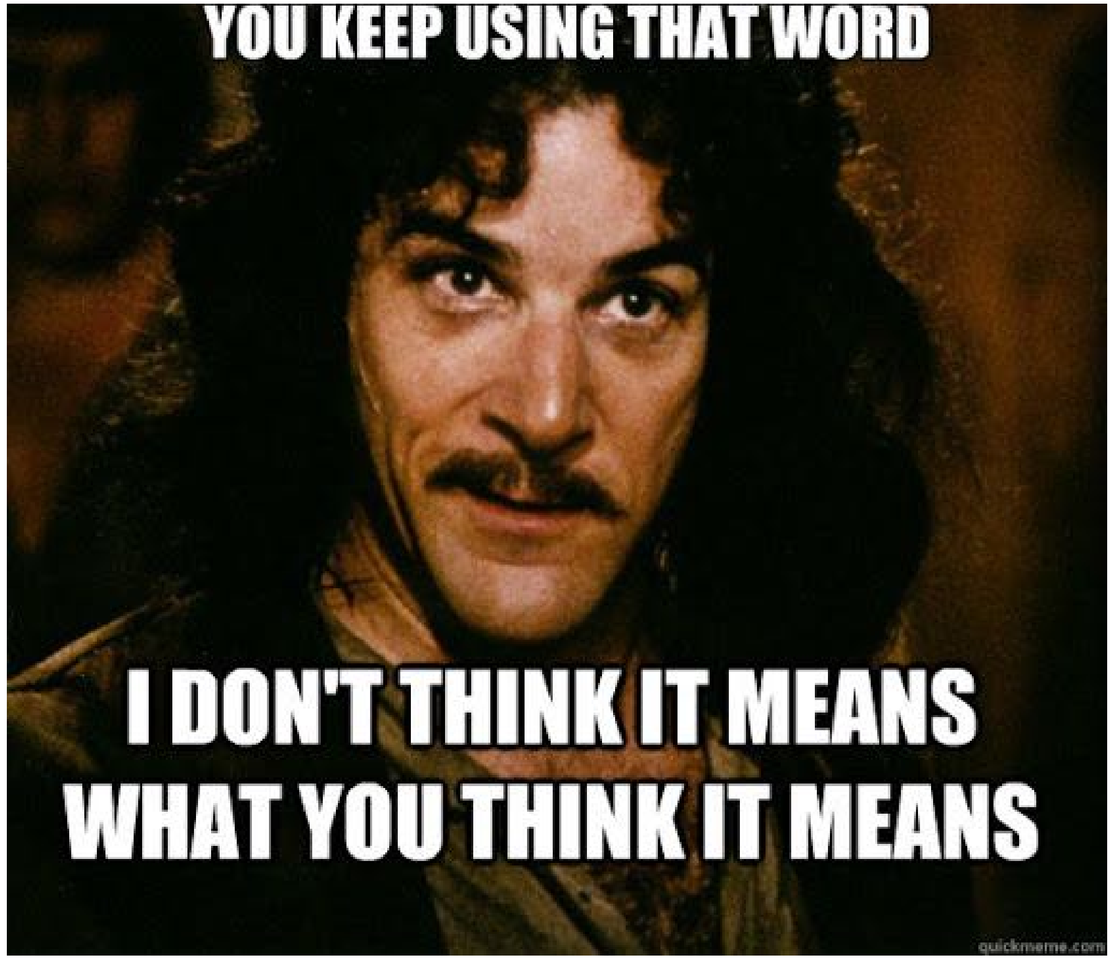

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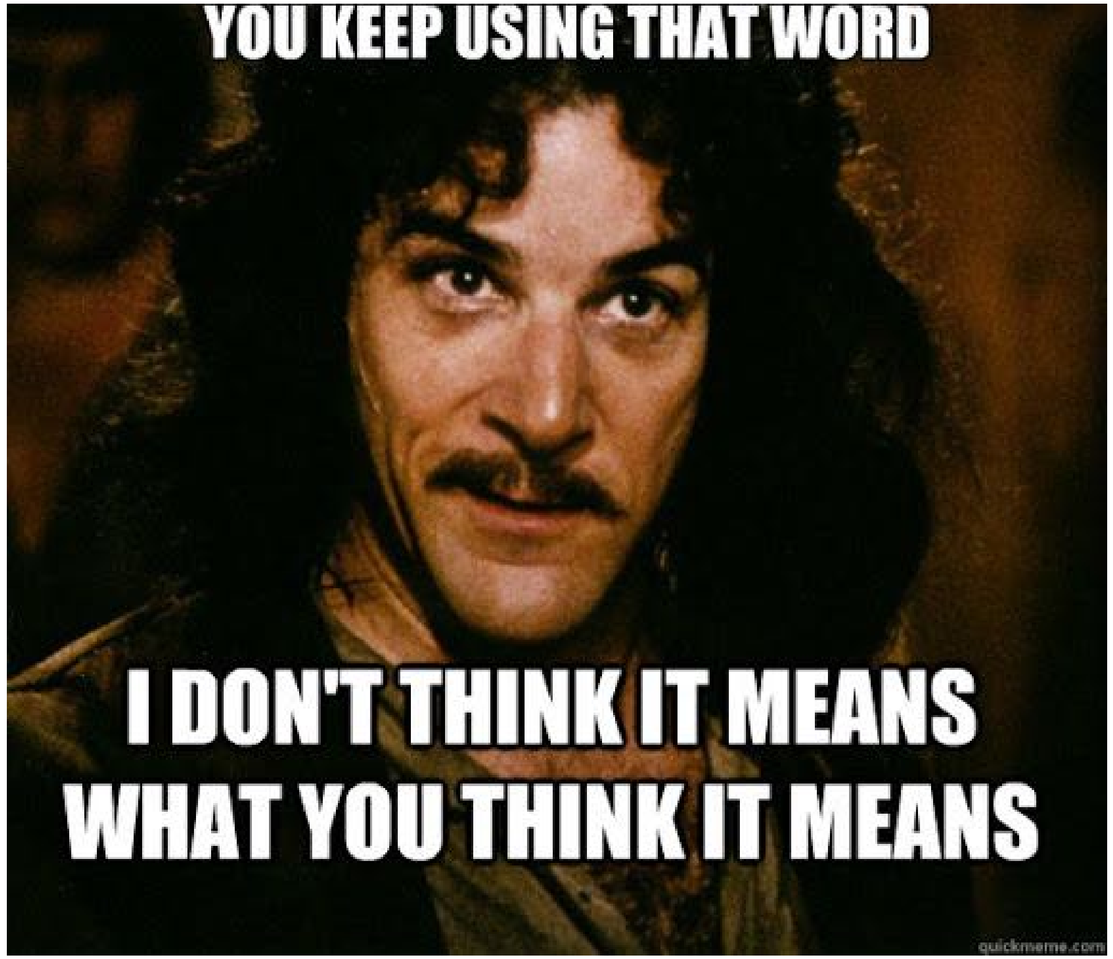

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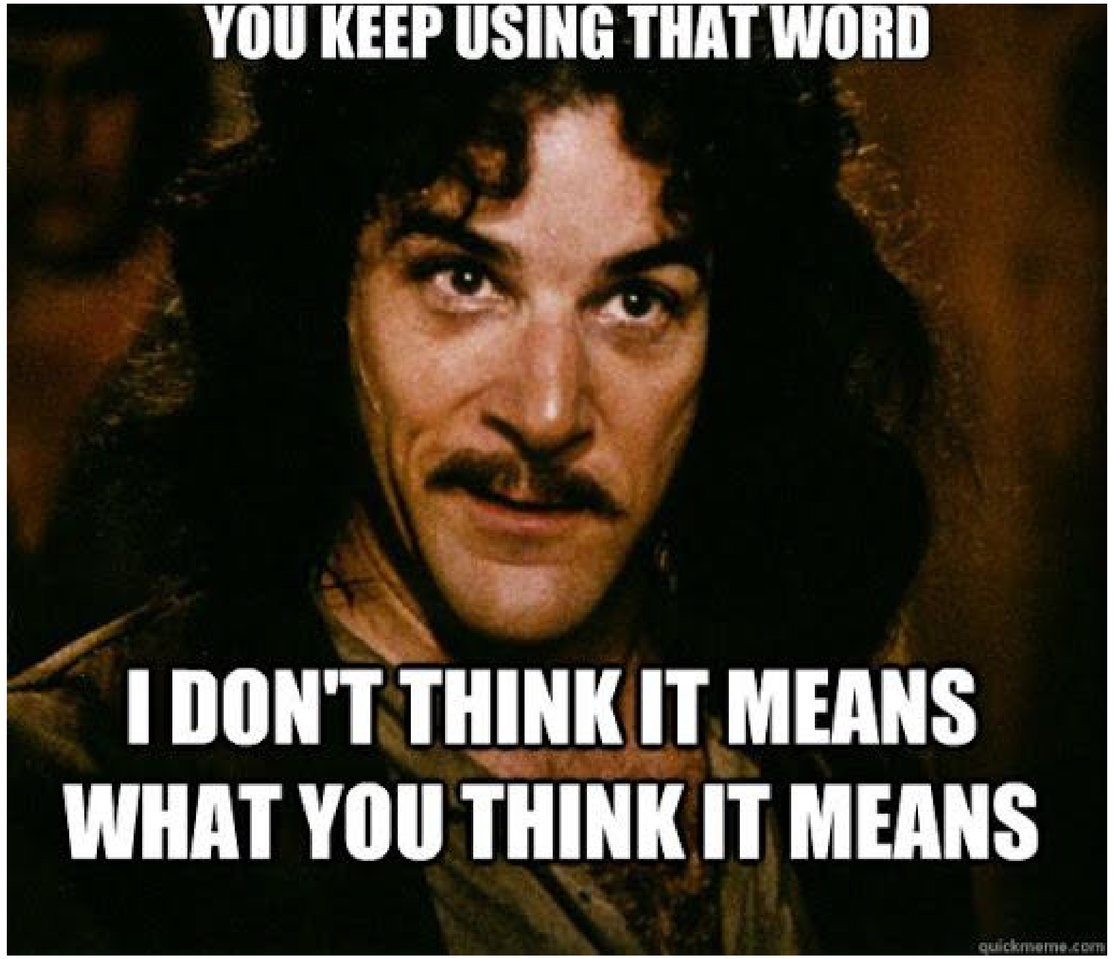

- Many fields: …robust statistics, robust control, robust optimization, adversarial robustness, robust learning…
- Robustness is a principle for decision-making

Optimization under undertainty

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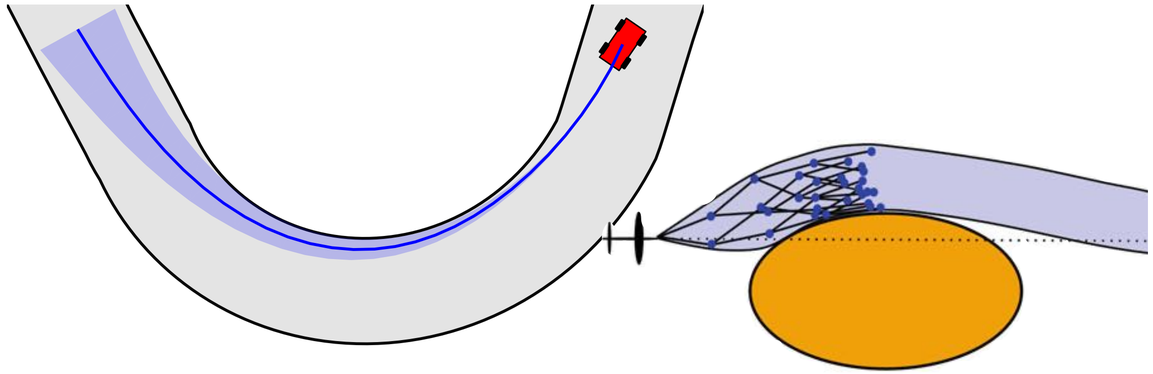

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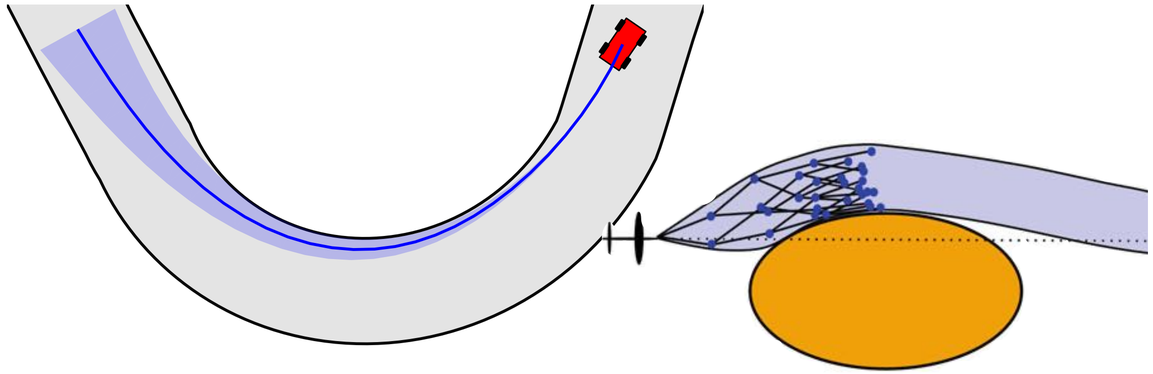

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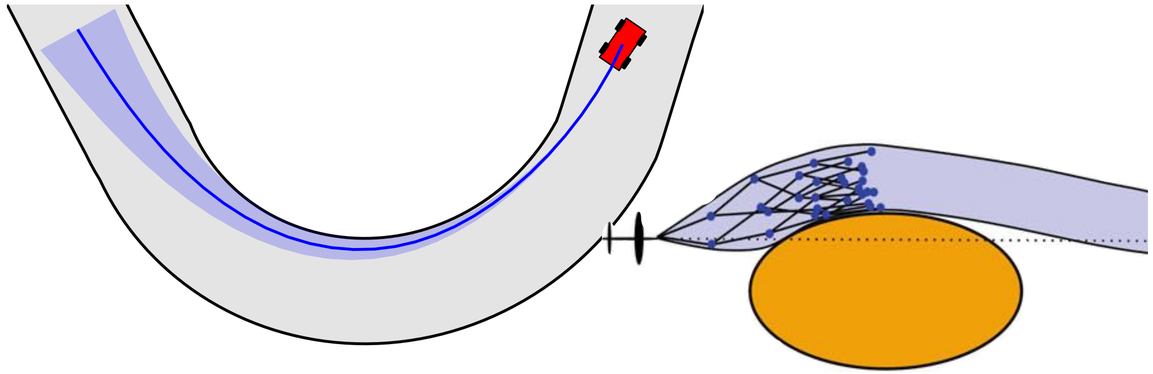

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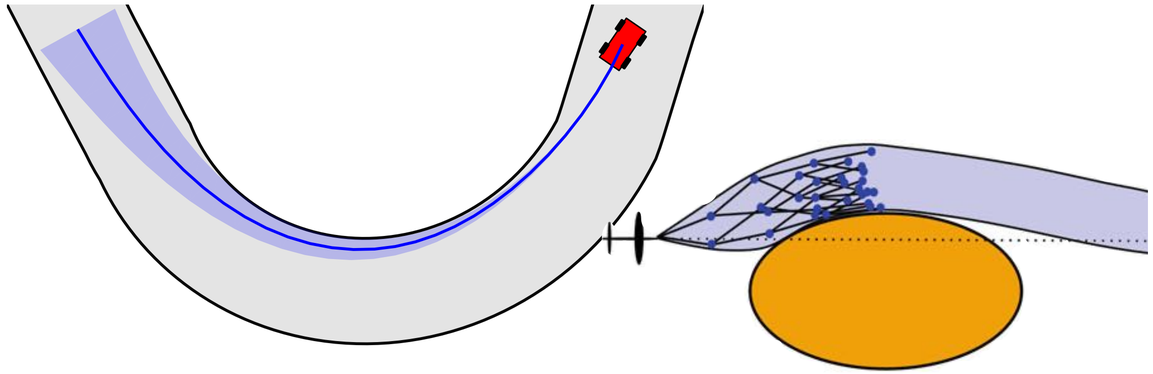

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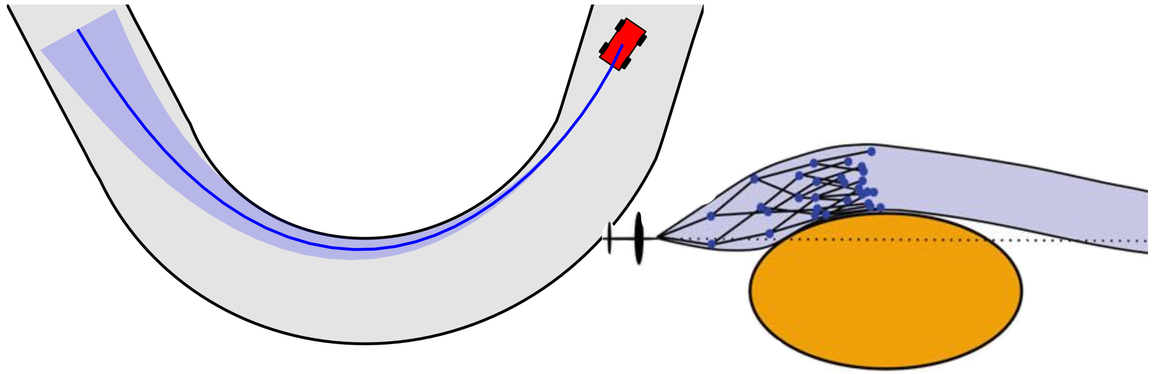

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- Do well in the worst case
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- Weakness: conservative — worst case doesn't often happen

Image credit: Mnih'13, MuJuCo, Houska and Villanueva '19, Hewing et al.'18

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$$\text{(D)} \min_{\theta} \hat{p}^T \theta + \epsilon \|\theta\|_2$$

  i.e., (P) = (D).

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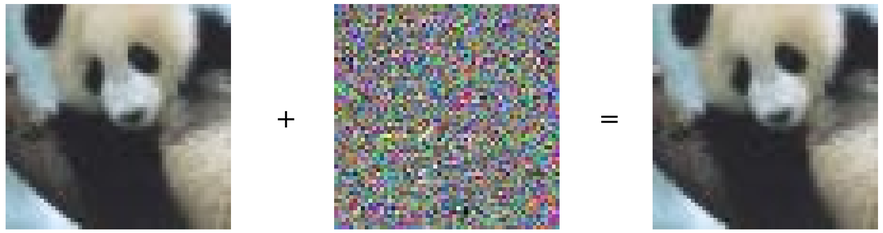

x $\quad$ δ

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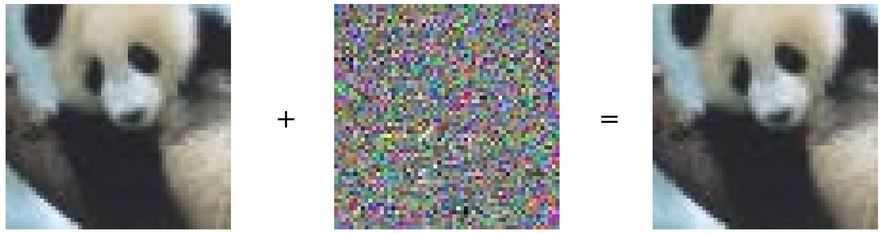

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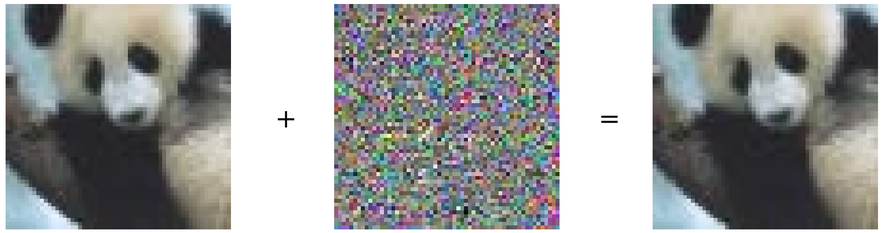

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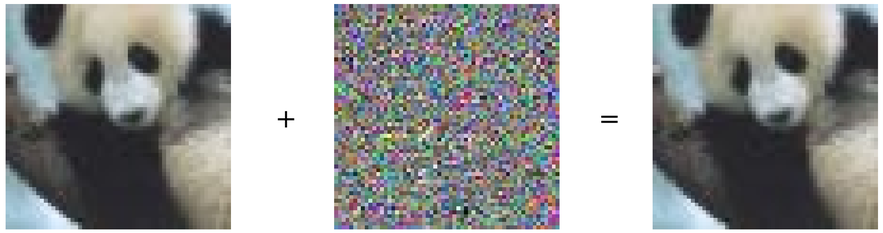

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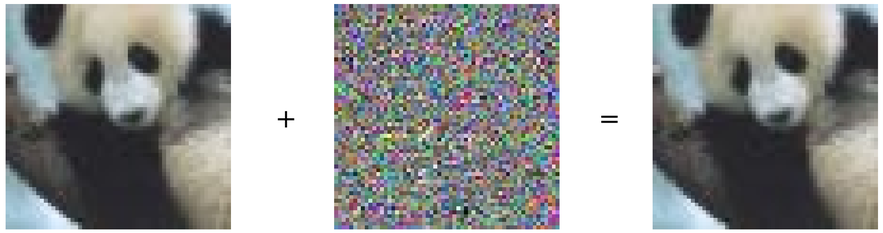

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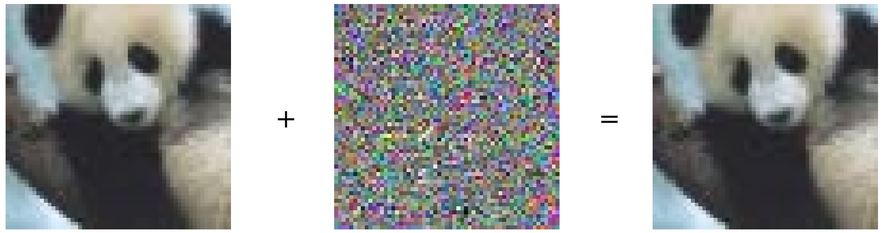

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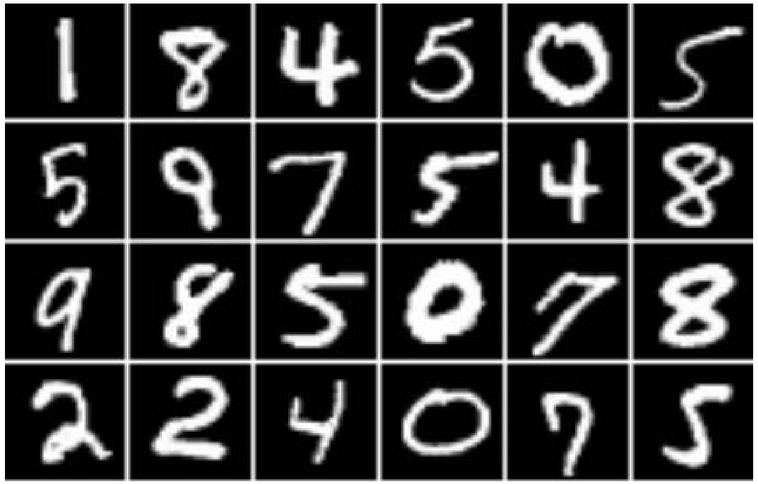
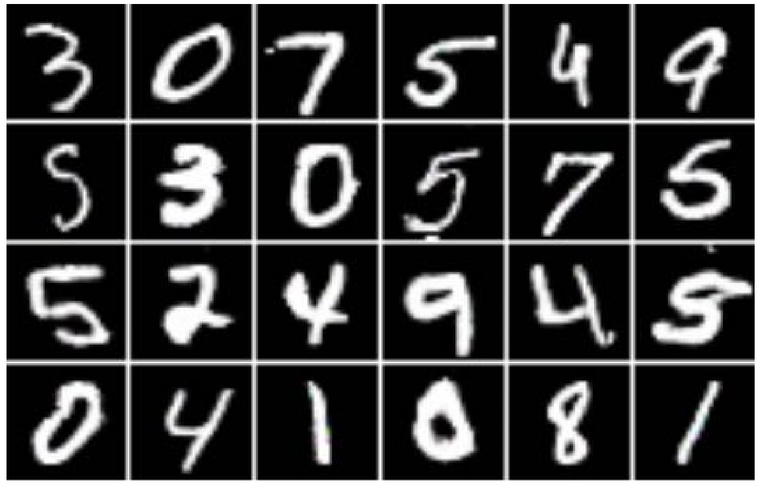
Image credit: Goodfellow et al. 2015

Distributional Robustness

How do we compare two sets of data?



Observed MNIST handwritten digits. X.

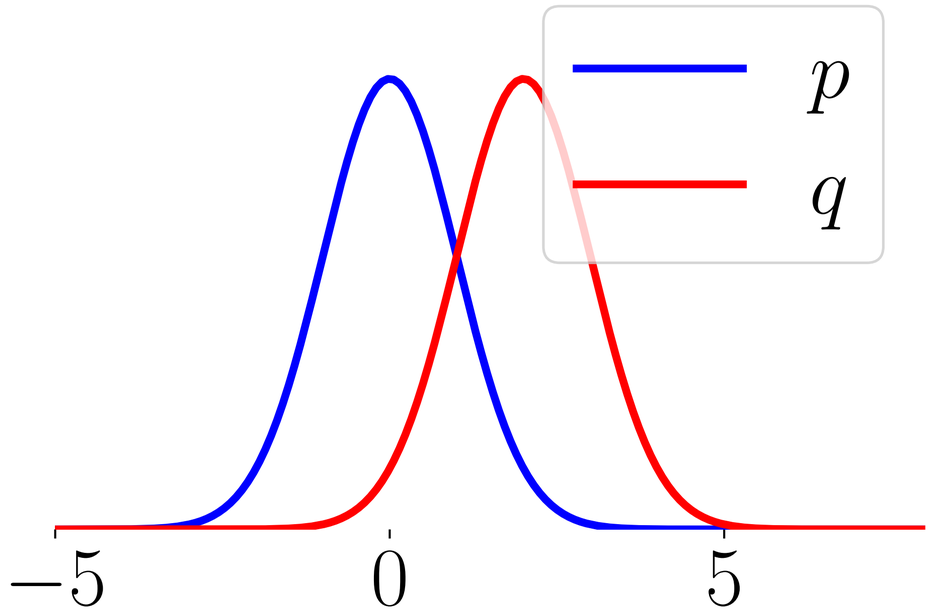


Generated images from a model. Y.

Is Y similar to X?

- Distance between distributions can be used to train generative models.

Case 1: Simple Mean Shift in 1D



- Two Gaussian distributions.

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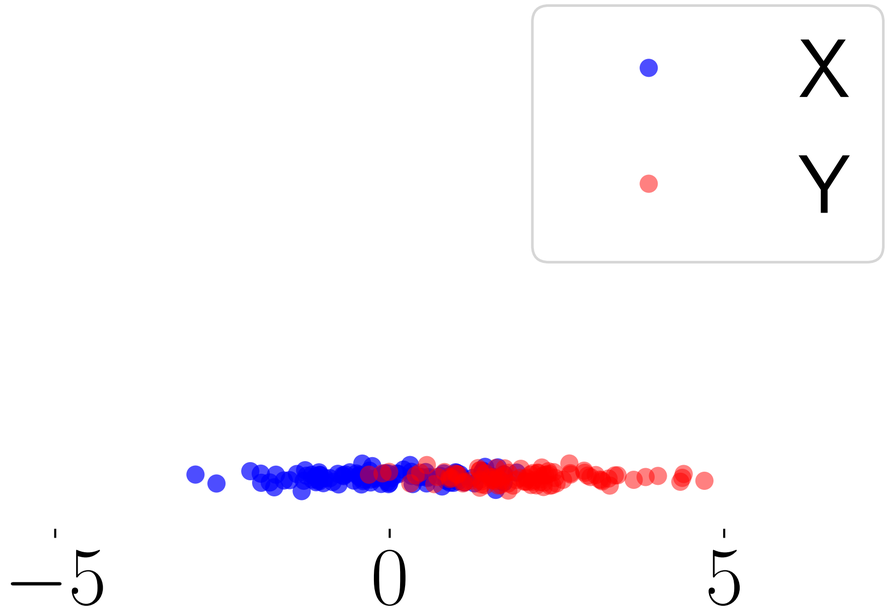

- We have only samples $\mathsf{X} \sim p$ and $\mathsf{Y} \sim q$.
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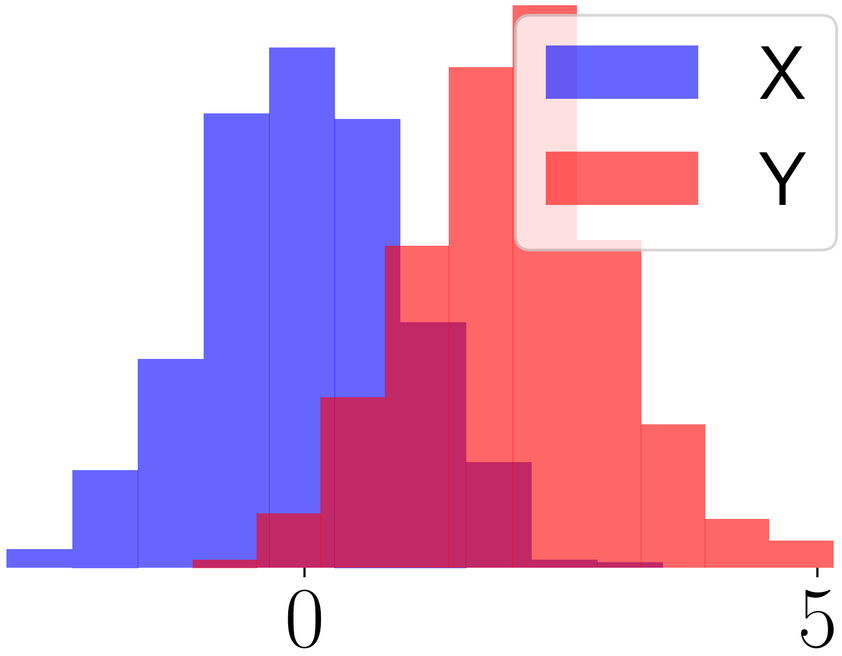

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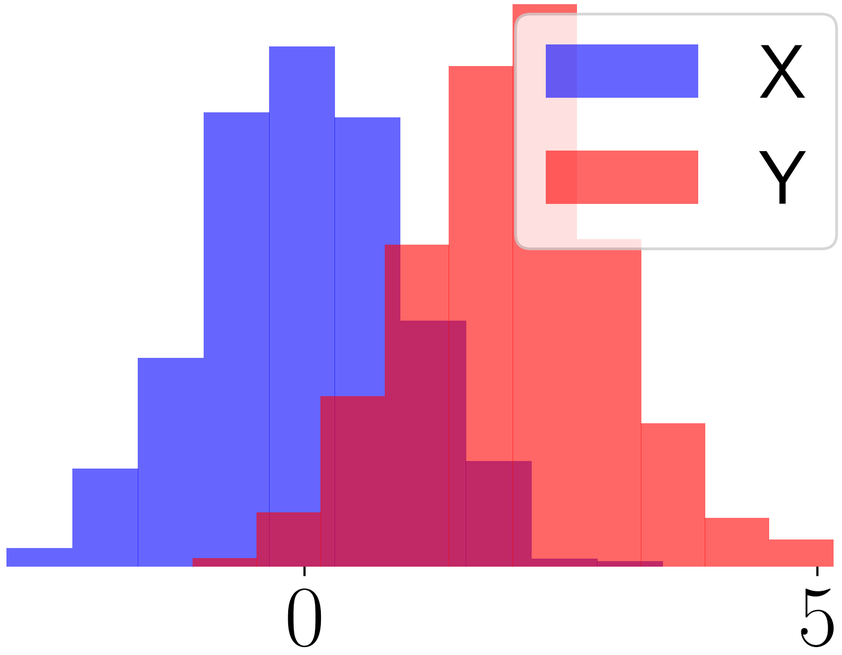
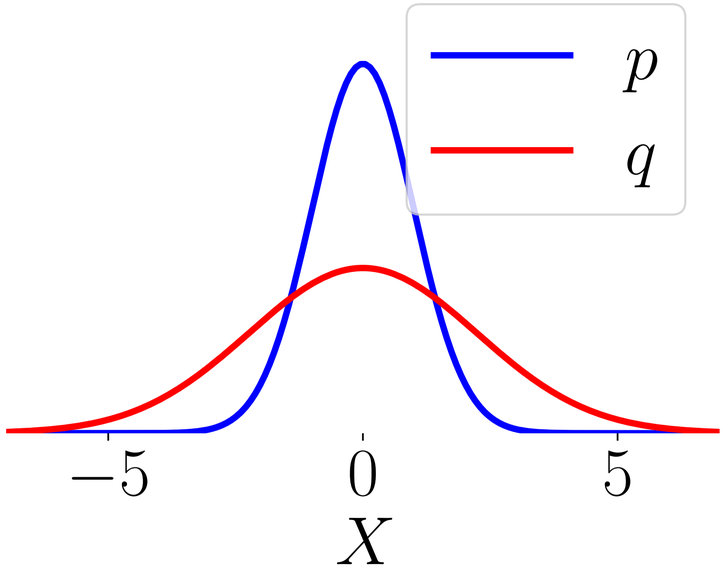


- Assume no differece in high-order moments.
- "Distance" = difference in the means. T-test.

$$\text{(population) } D_1(p, q) := |\mathbb{E}_{X\sim p}[X] - \mathbb{E}_{Y\sim q}[Y]|$$

$$\text{(empirical) } \hat{D}_1(\mathsf{X}, \mathsf{Y}) = \left|\frac{1}{n}\sum_{i=1}^{n} x_i - \frac{1}{n}\sum_{j=1}^{n} y_j\right|$$

Case 2: Same Mean, Different Variances



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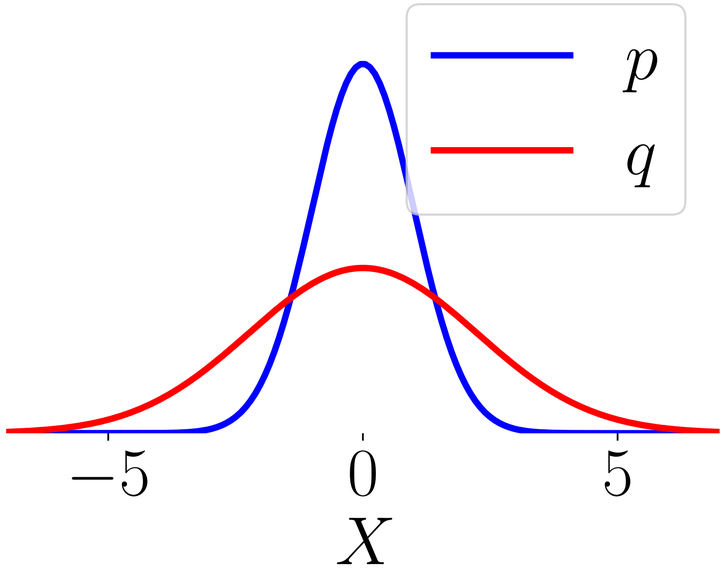

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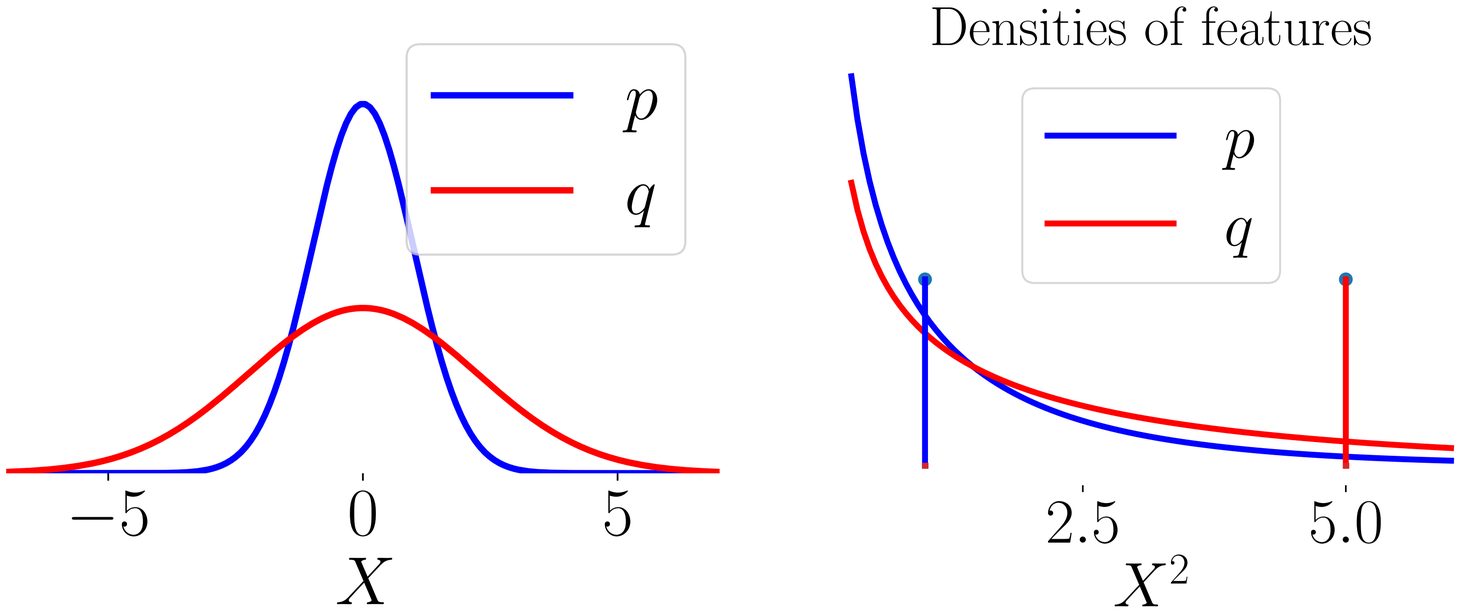

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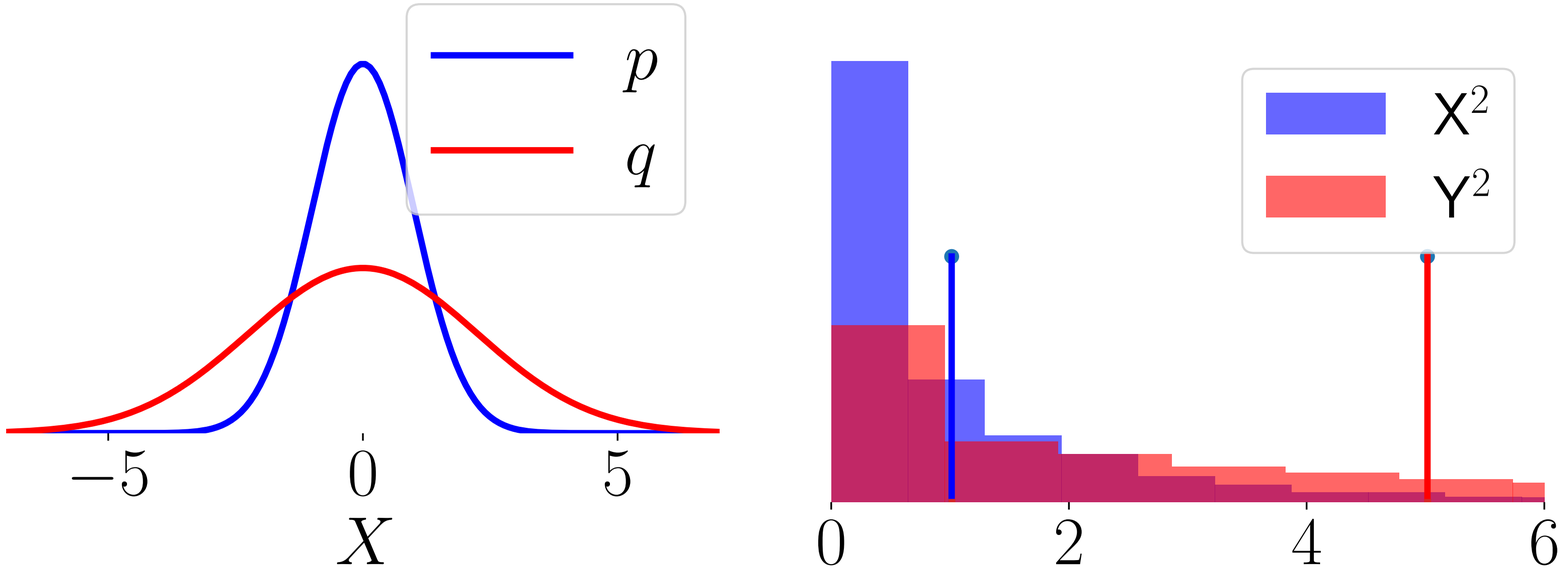

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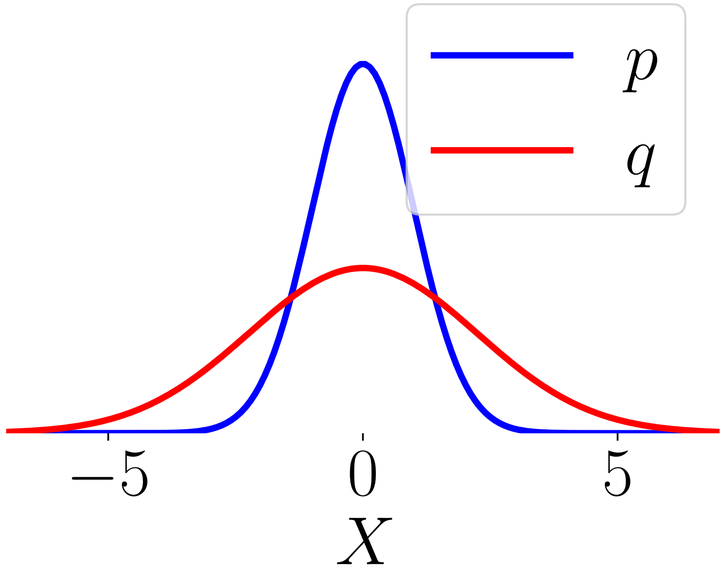

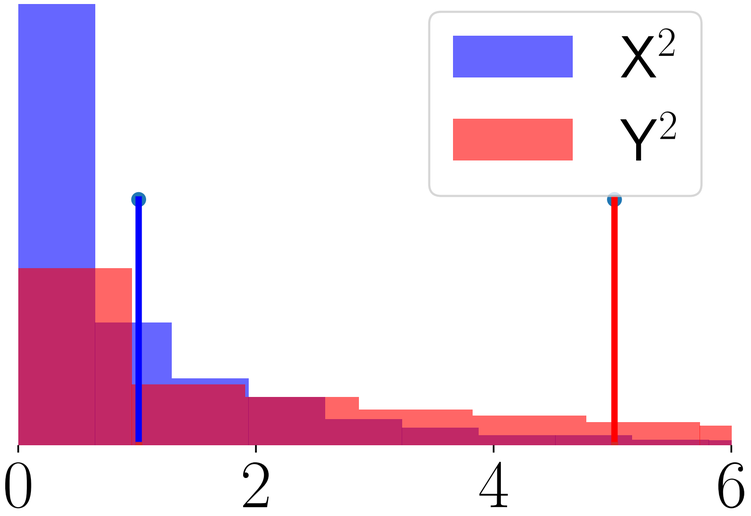

- $D_1(p, q) := |\mathbb{E}_{X\sim p}[X] - \mathbb{E}_{Y\sim q}[Y]|$ cannot detect the difference. Why?
- **Idea**: look at difference in means of features $\phi(\cdot)$ of X and Y.
- New "distance":

$$D_2(p, q) = \left\|\mathbb{E}_{X\sim p}[\phi(X)] - \mathbb{E}_{Y\sim q}[\phi(X)]\right\|,$$

where $\phi(x) = (x, x^2)^\top$.

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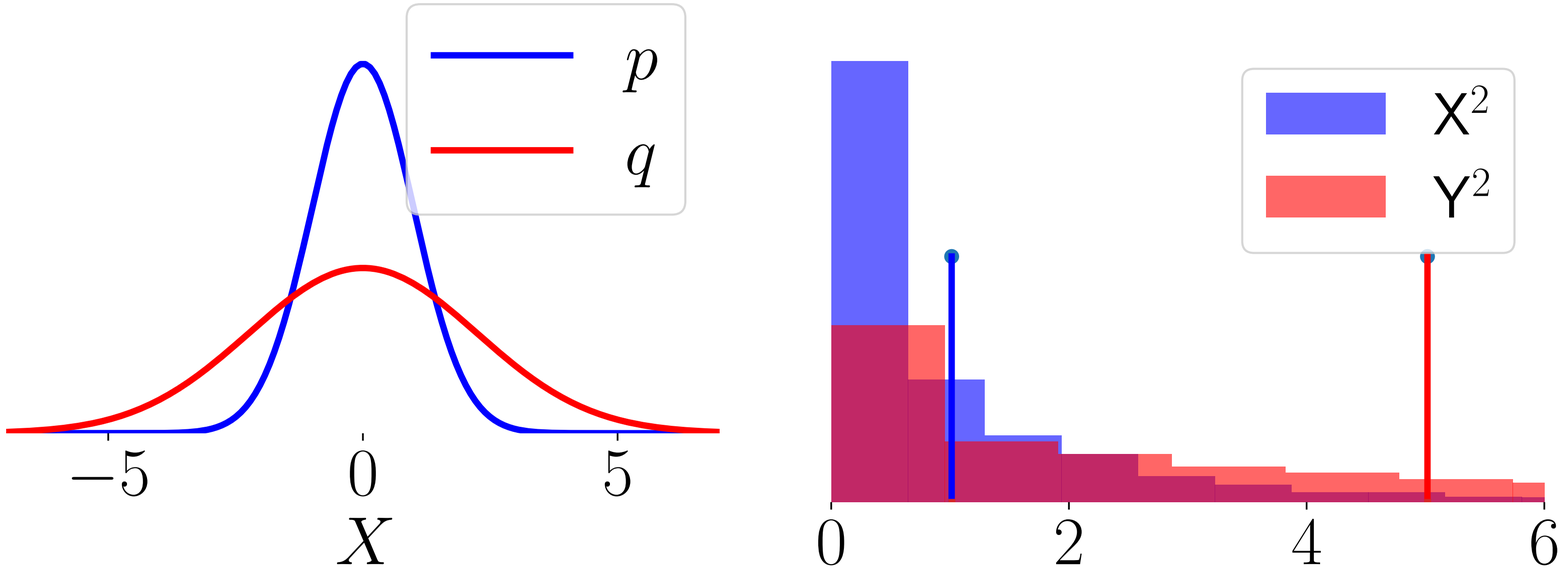

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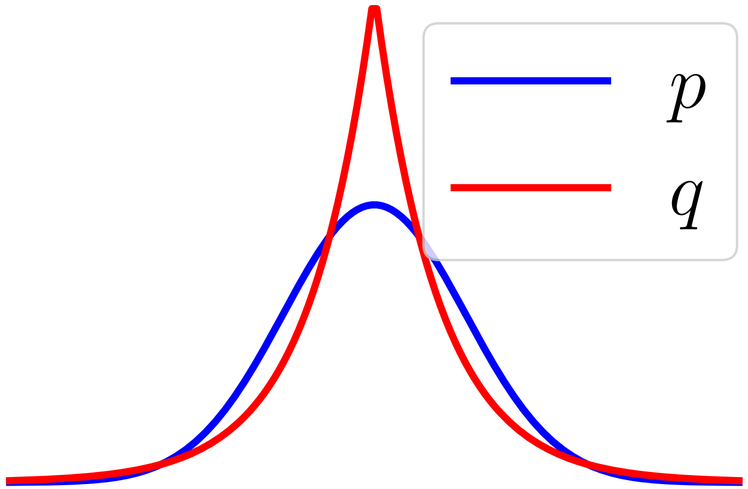
Case 3: Difference in High-Order Moments



- p = Gaussian distribution,
  q = Laplace distribution.
- Same mean **and** variance.
- D_2 fails.

- $\phi(x) = (x, x^2, x^4)^\top$ works. Difference is in kurtosis (4^{th} moment).
- $\phi(x) = (x, x^2, x^4, \cos x, e^x, \ldots)^\top$. But, when to stop?
- **Solution**: Use an infinite-dimensional feature map $\phi(\cdot)$ with the kernel trick.

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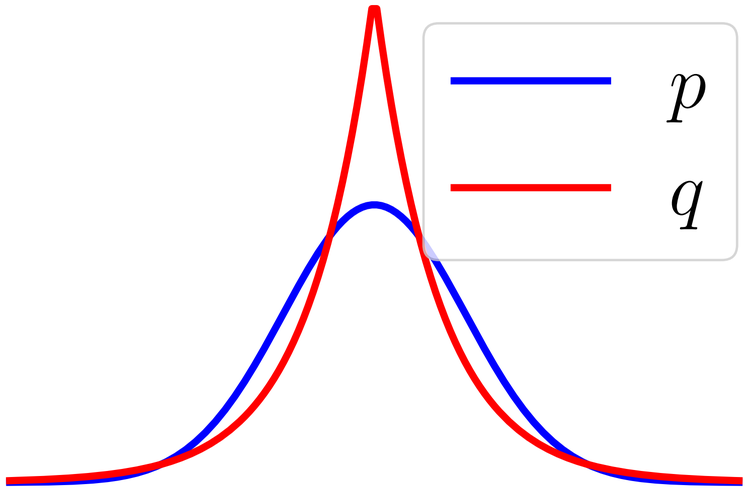

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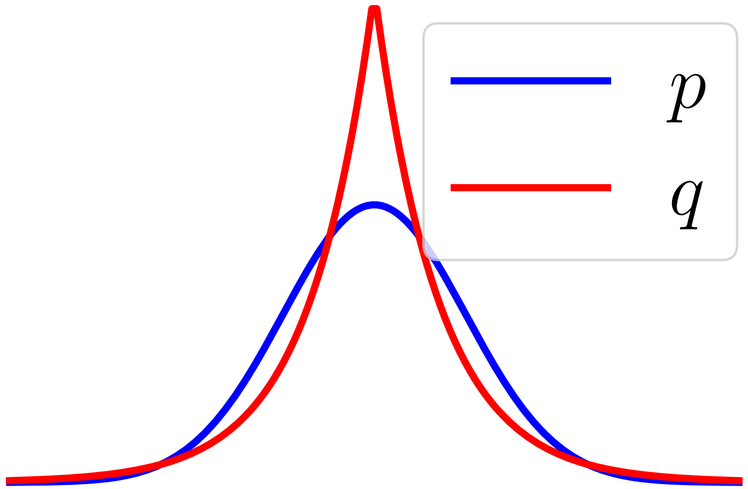

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Working with probability measures

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The probability “simplex” $\mathscr{P}$

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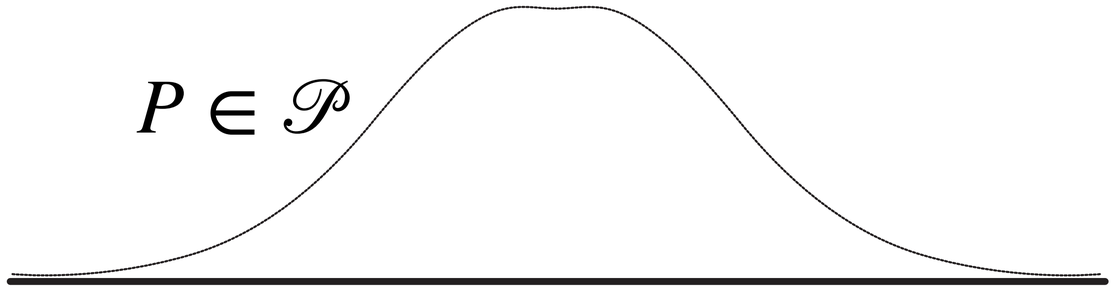

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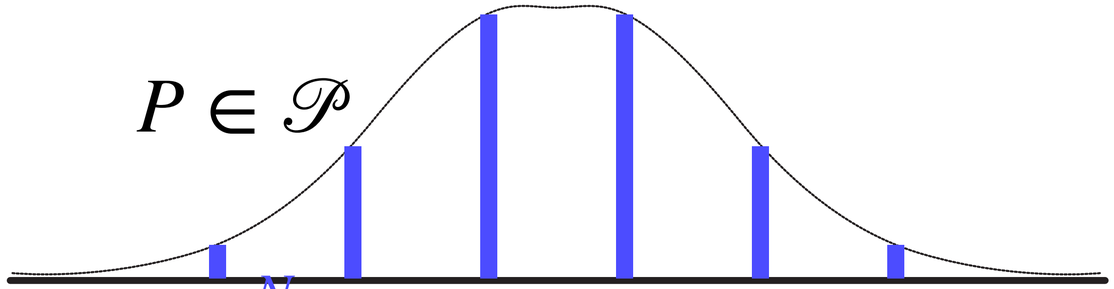

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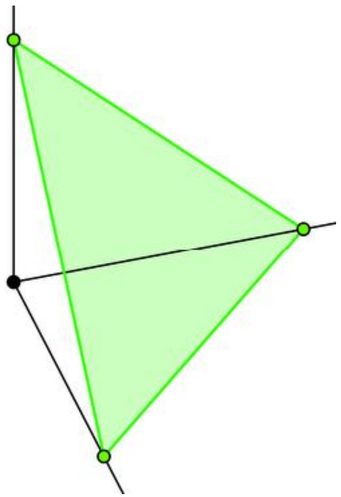

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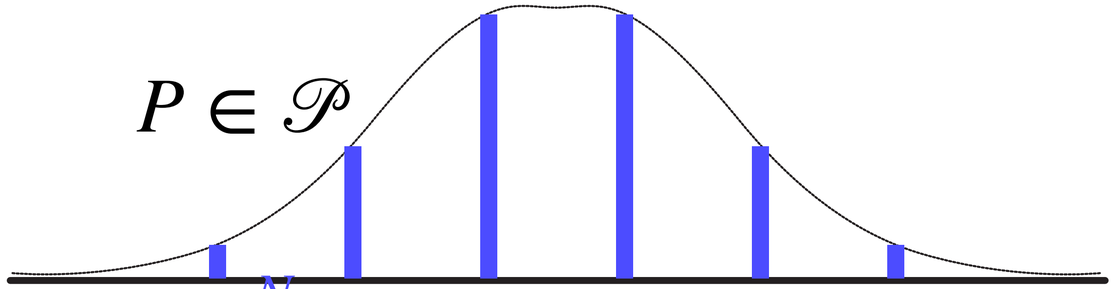

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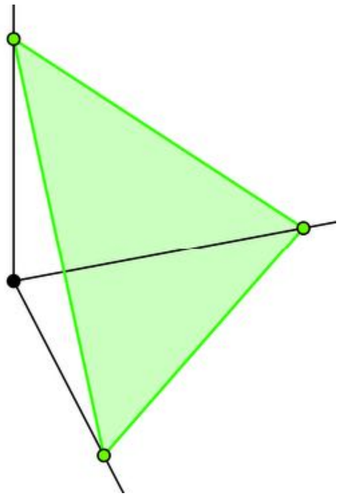

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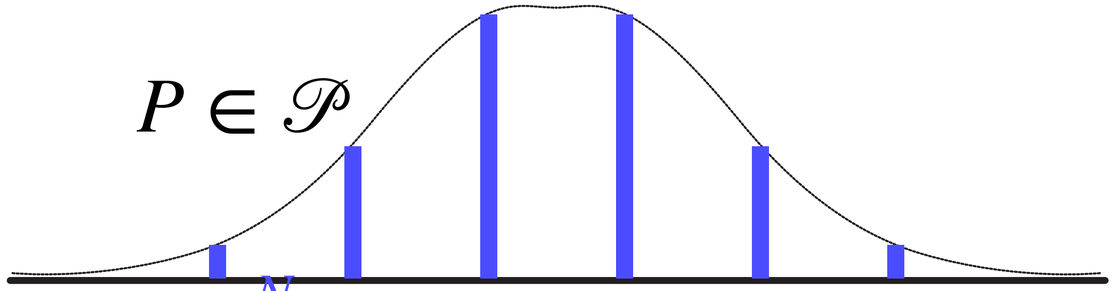

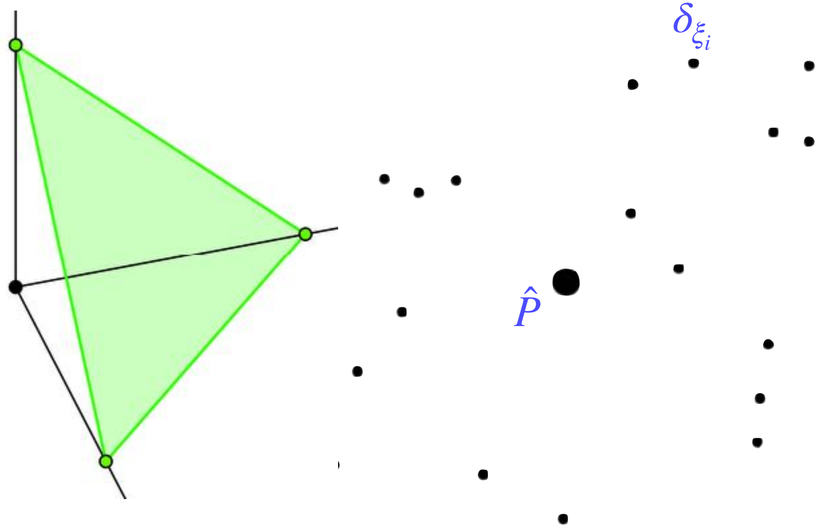

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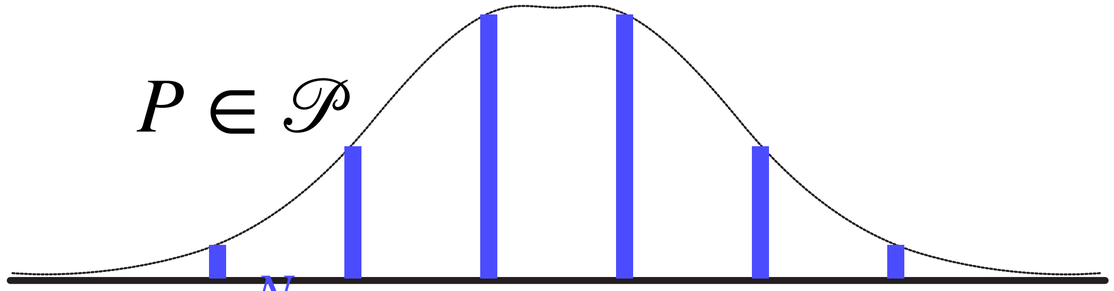

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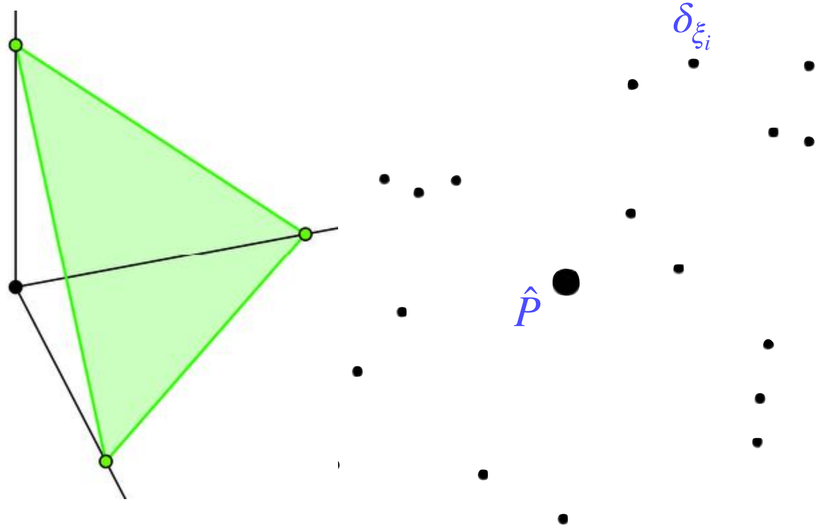

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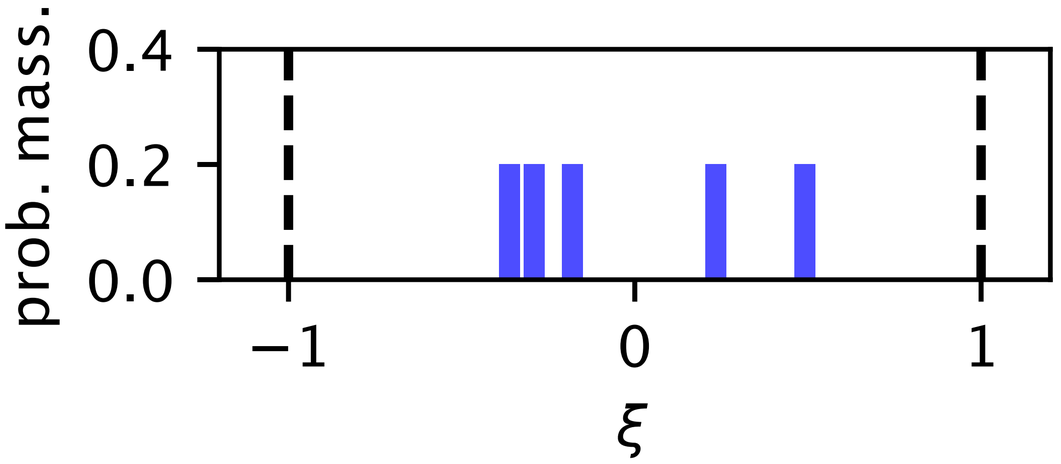

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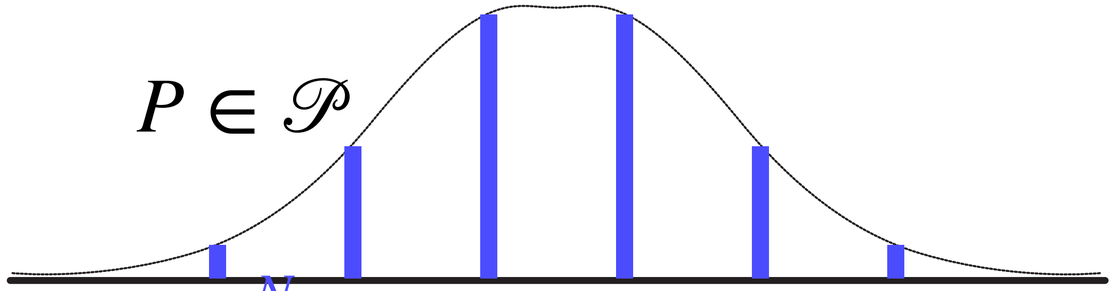

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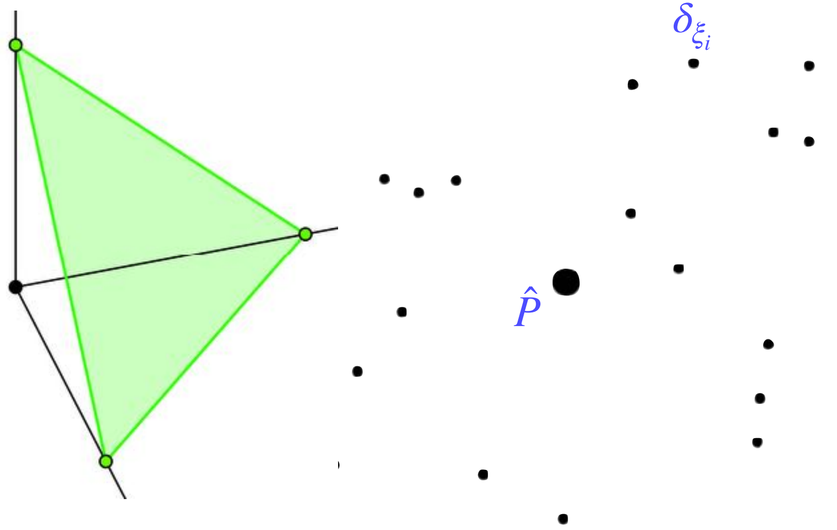

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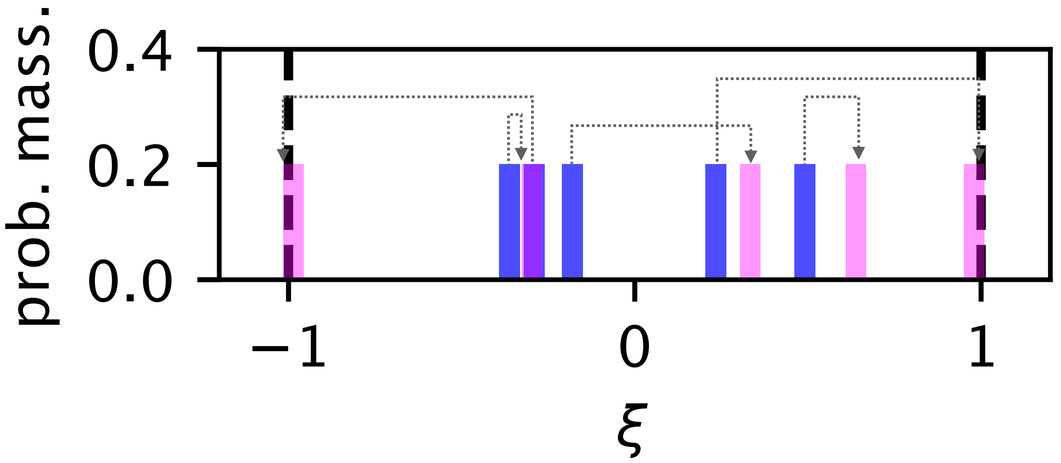

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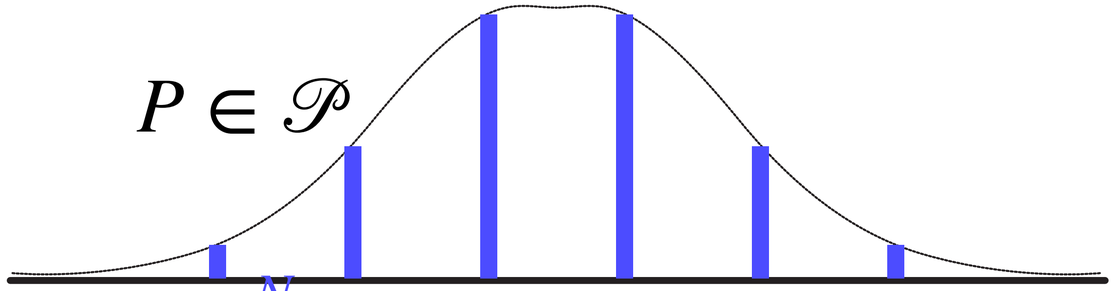

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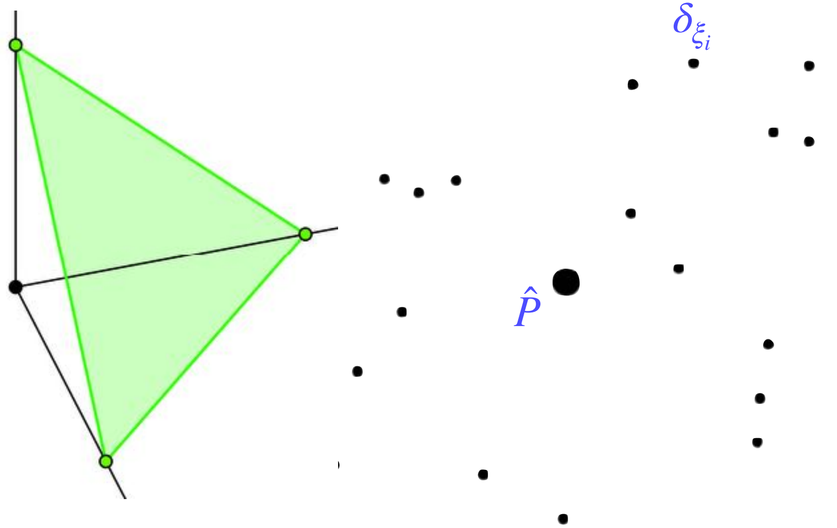

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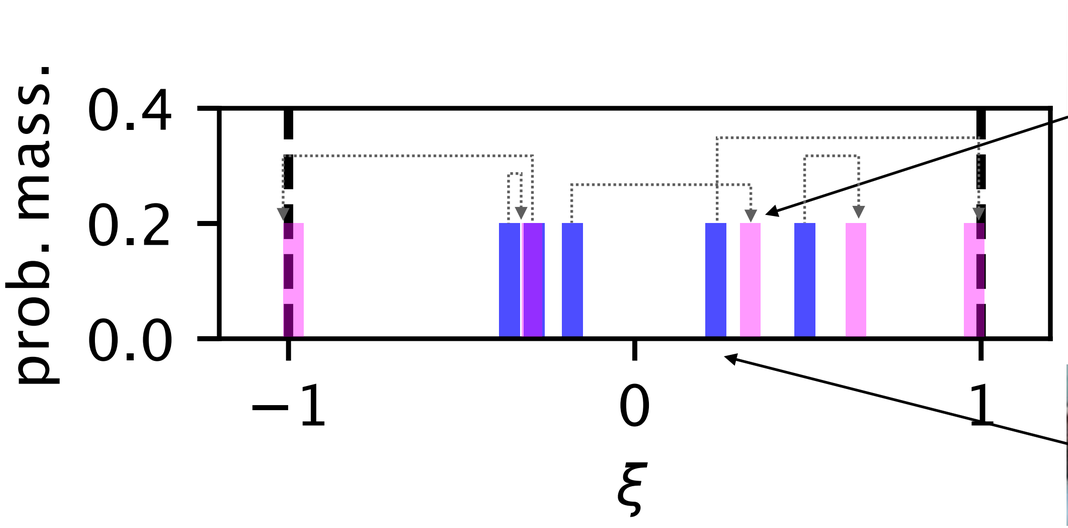

Adversarial attack: Goodfellow et al. 2015

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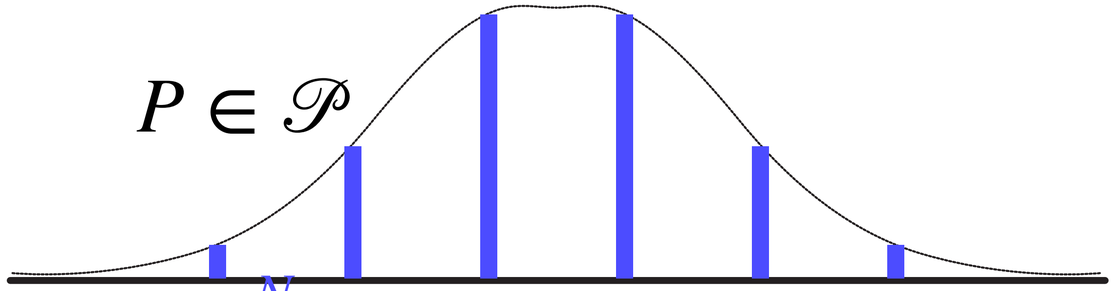

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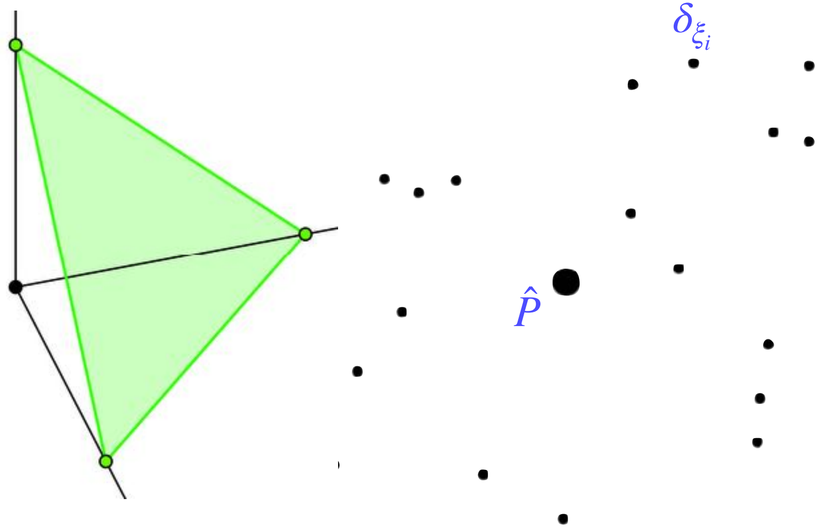

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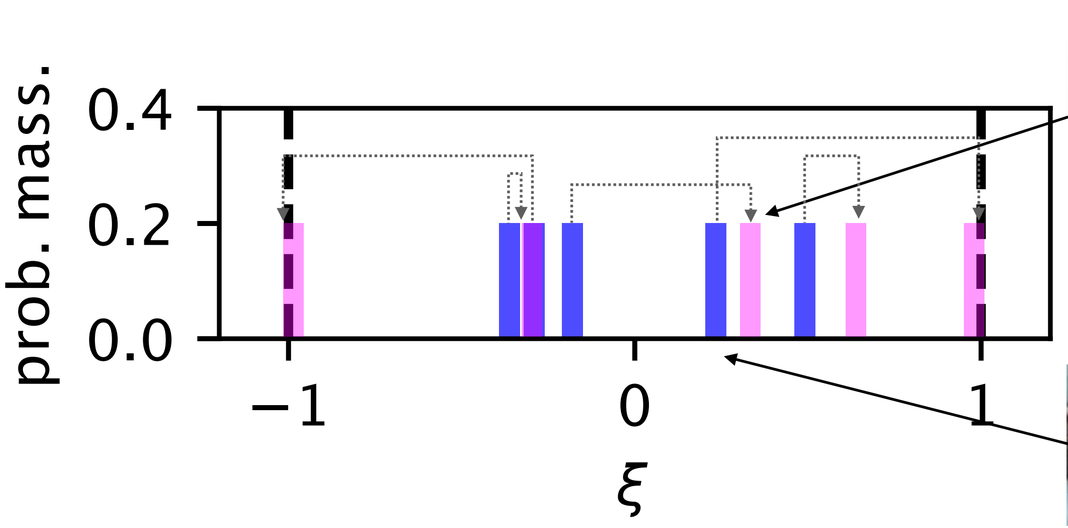

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P might only differ slightly from $\hat{P}$, but can break the system.

Wasserstein distance

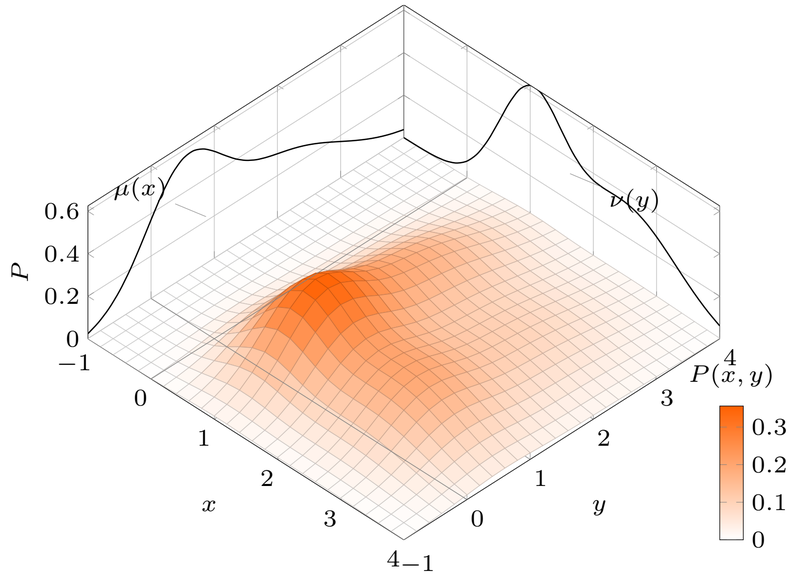
The optimal value of the Kantorovich problem

$$\mathcal{W}_p(P,Q) = \inf_{\pi \in \Pi(P,Q)} \left\{ \int \|u-v\|^p \, d\pi(u,v) \right\}^{1/p}$$

where $p \geq 1$, π is a *t*ransport plan (coupling) that belongs to the set of valid plans

$$\Pi(\mu,\nu) = \{\pi \in P(X \times X) : (\pi_0)_{\#}\gamma = \mu, (\pi_1)_{\#}\gamma = \nu, \}.$$

π_0 and π_1 are the two projections onto the marginal distributions.



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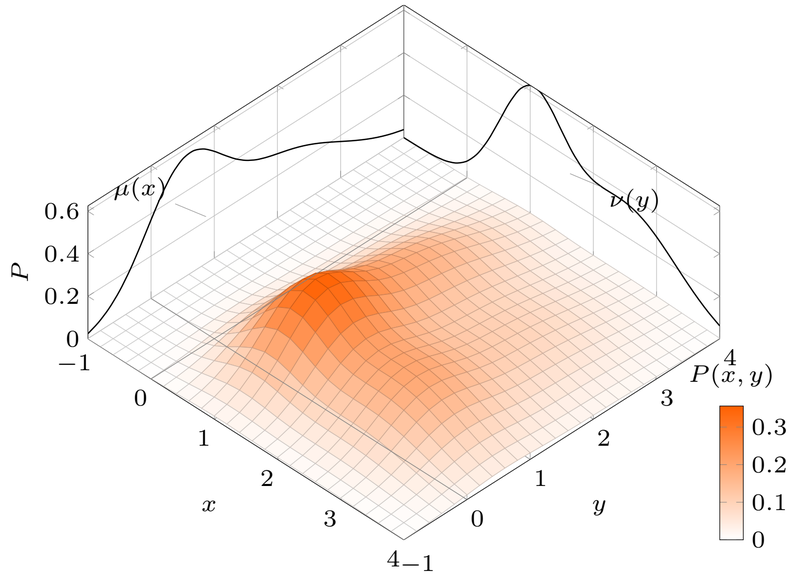

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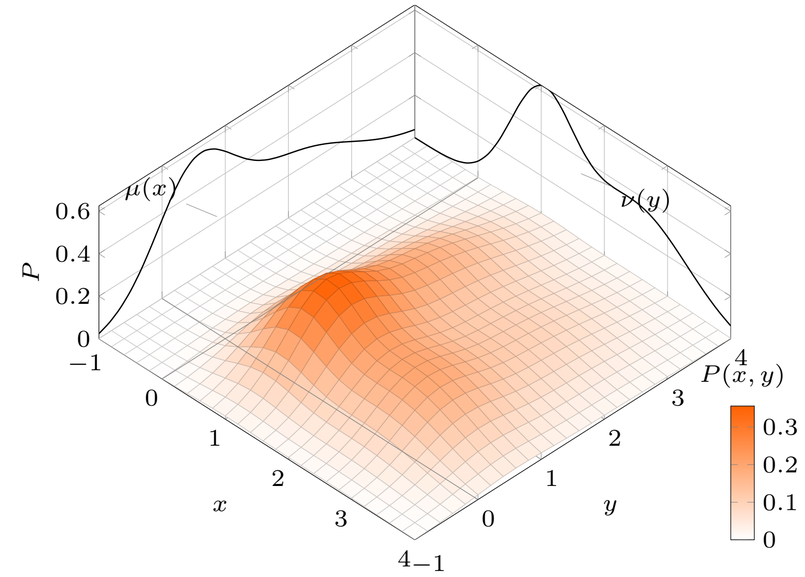

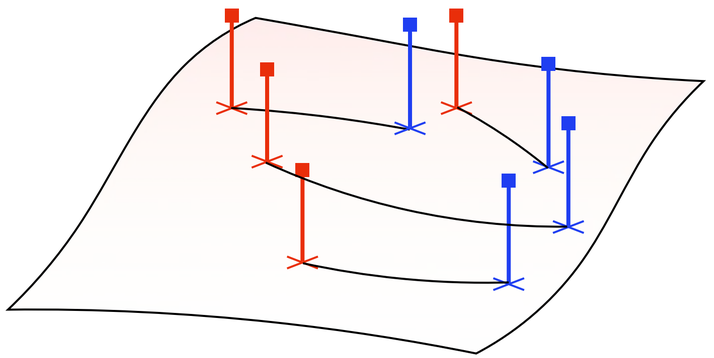

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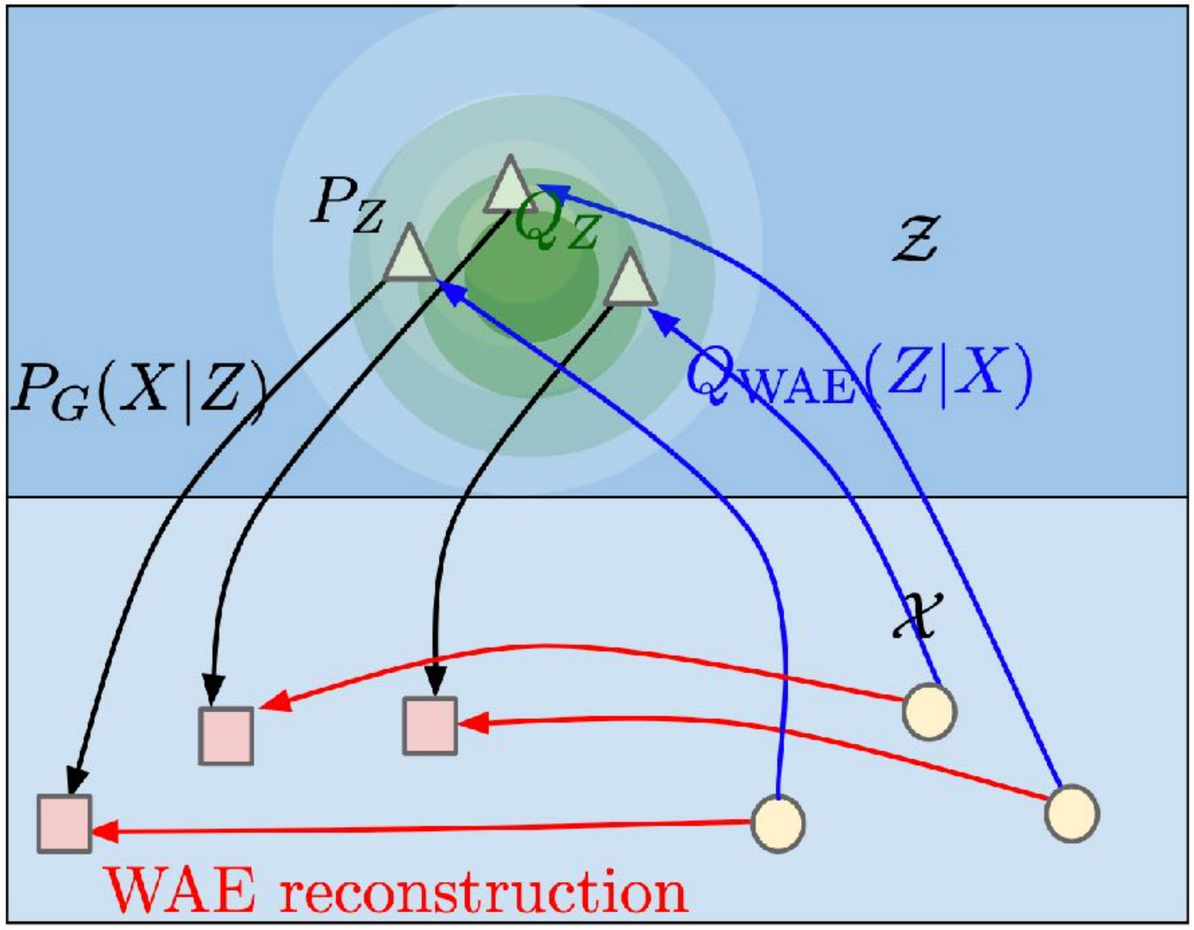

Learning with kernels (the modern way)

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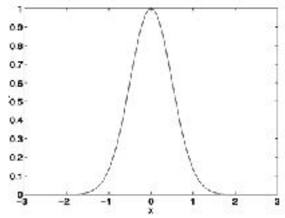

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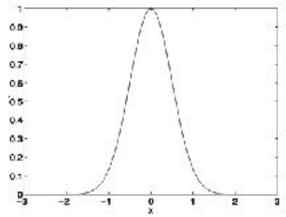

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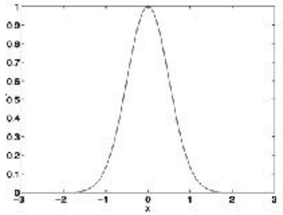

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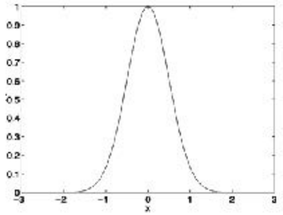

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$\mathcal{P} \quad \mu_P := \int \phi \, dP$

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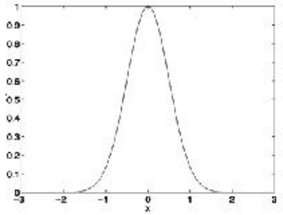

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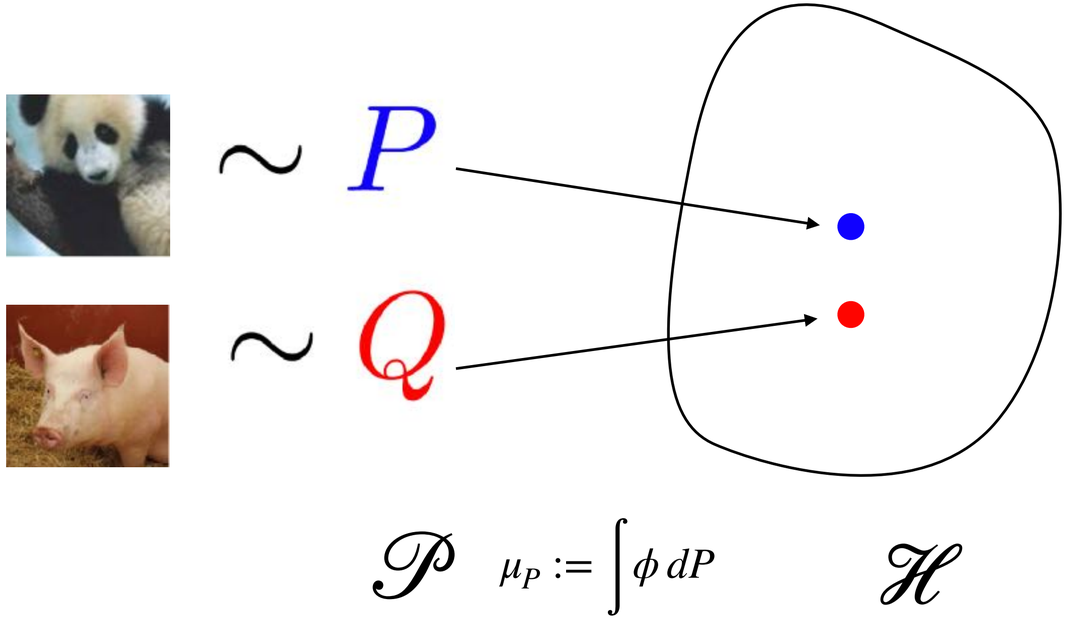

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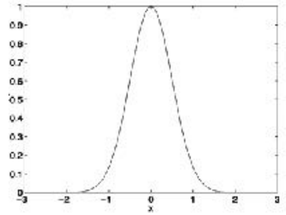

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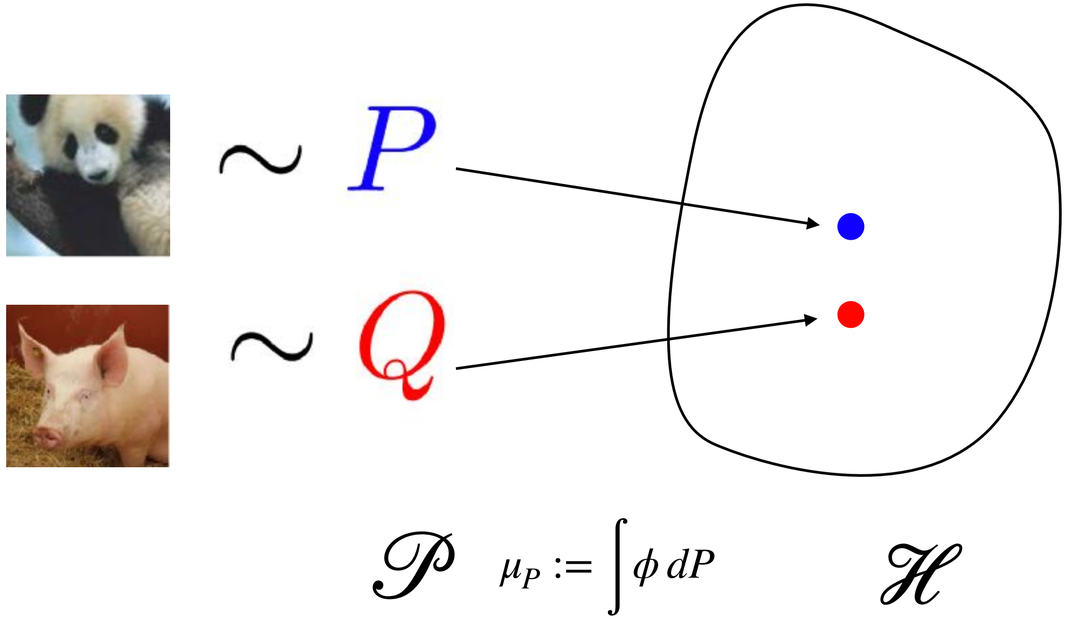

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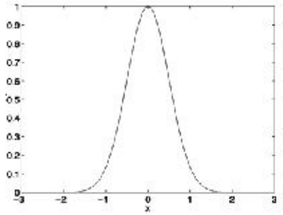

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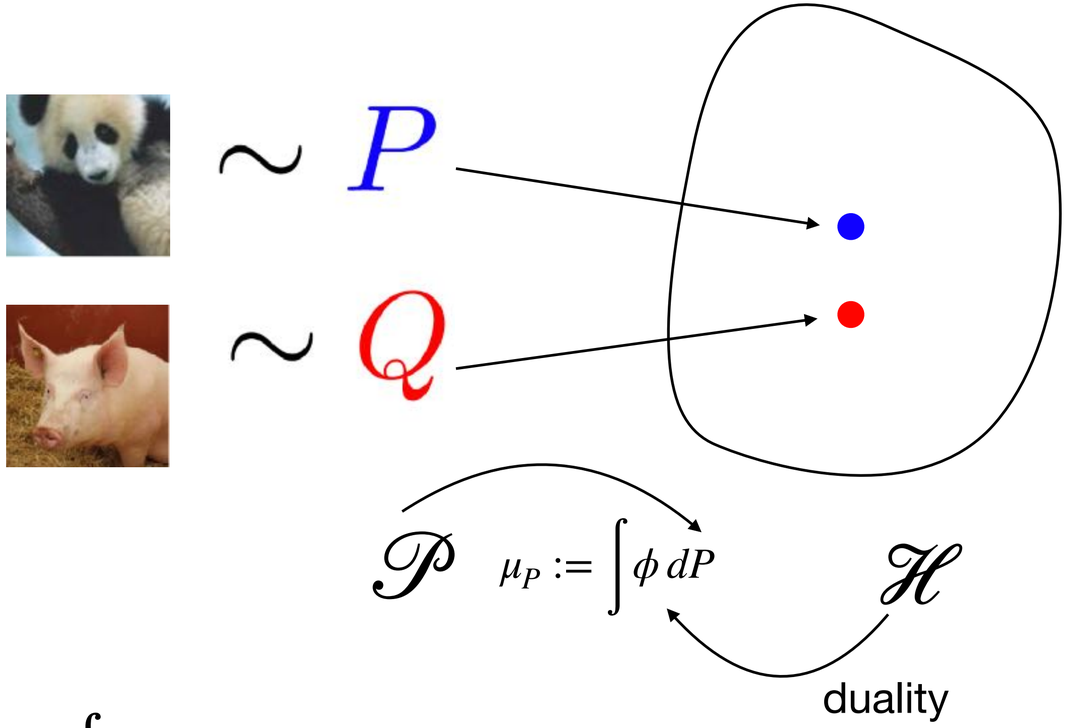

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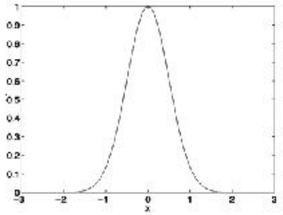

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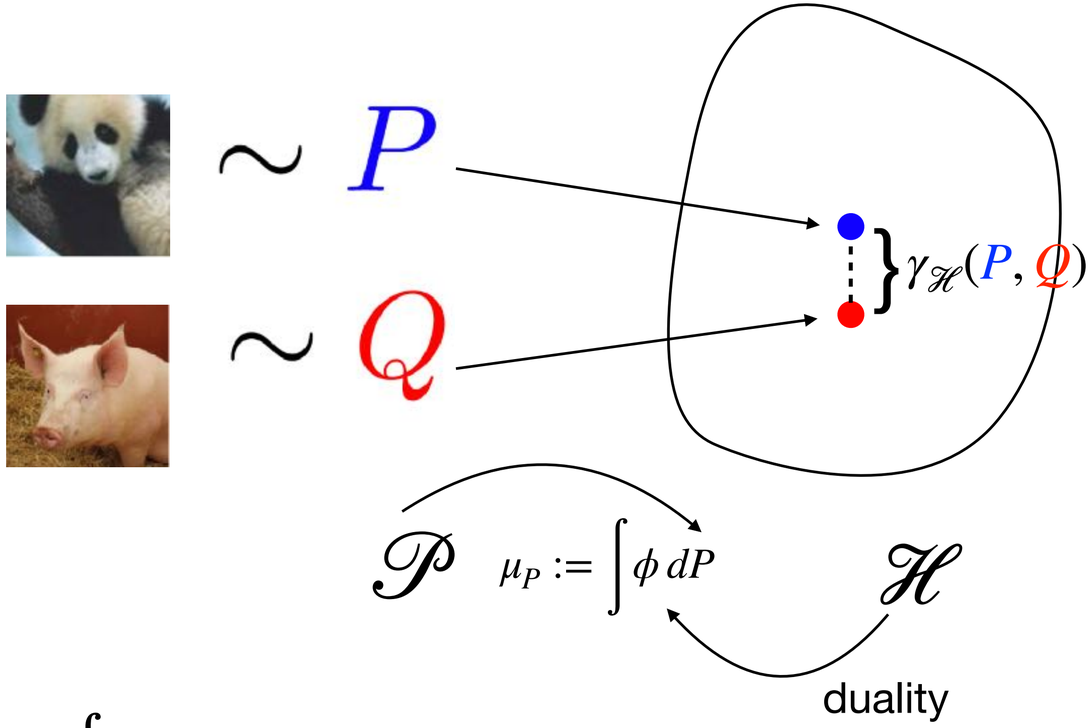

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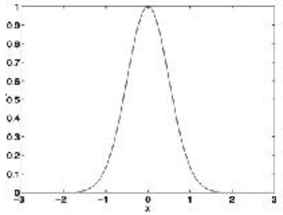

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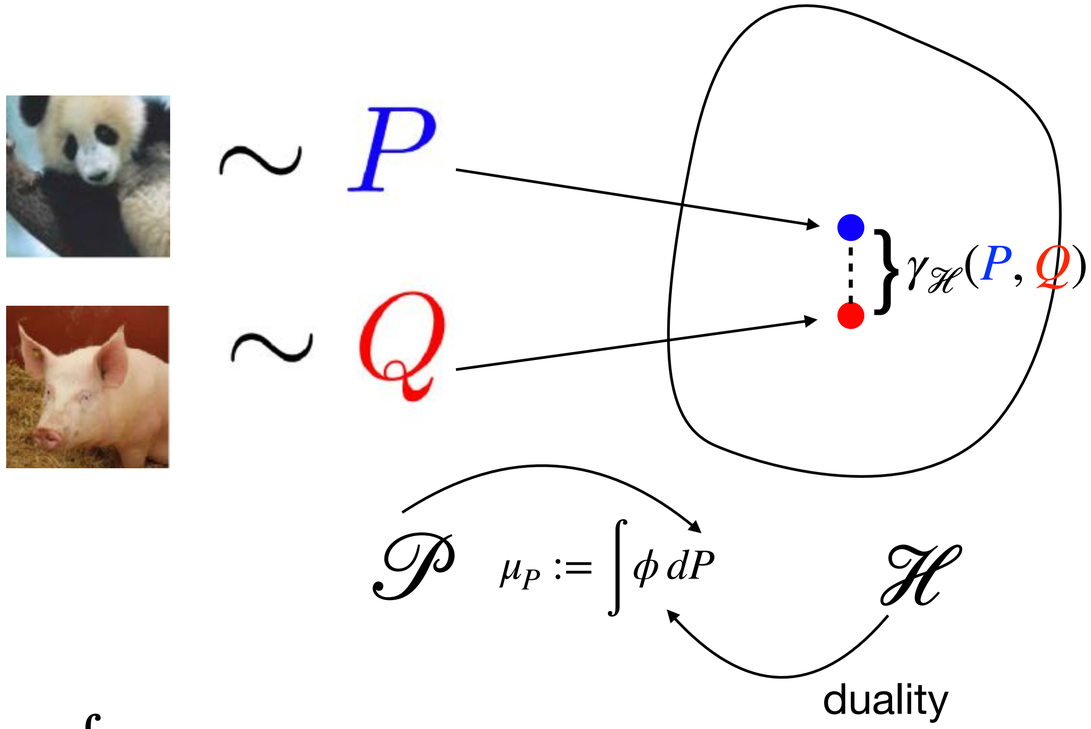

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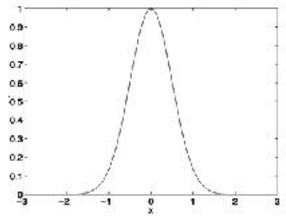

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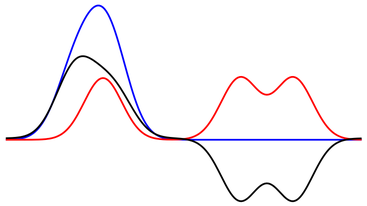

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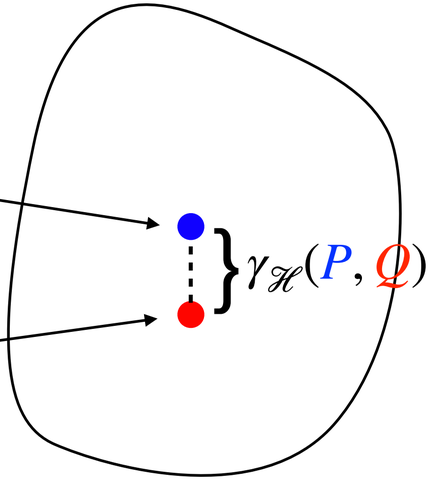

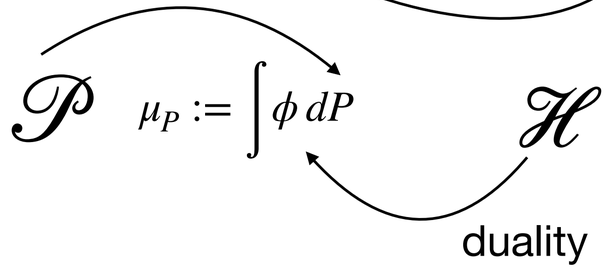

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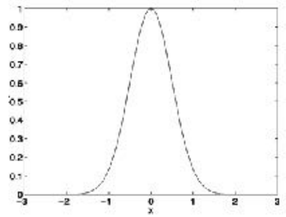

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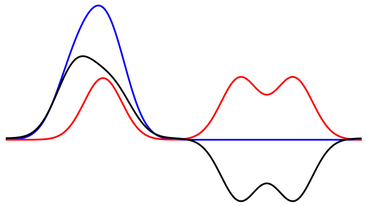

  - Special cases:
    $\mathcal{F} = \{f : \|f\|_{\mathcal{H}} \leq 1\}$ –> Maximum Mean Discrepancy (MMD)
    $\mathcal{F} = \{f : \|f\|_{\text{lip}} \leq 1\}$ –> Wasserstein (type-1)

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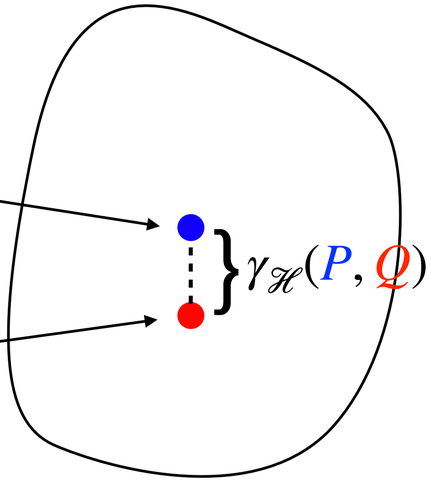
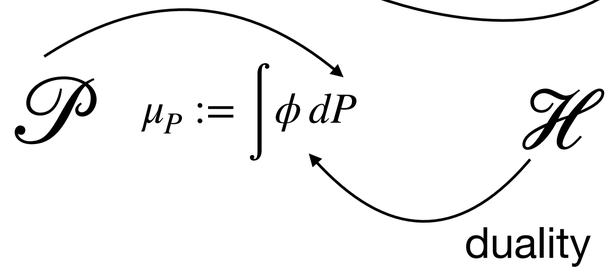
$\sim Q$





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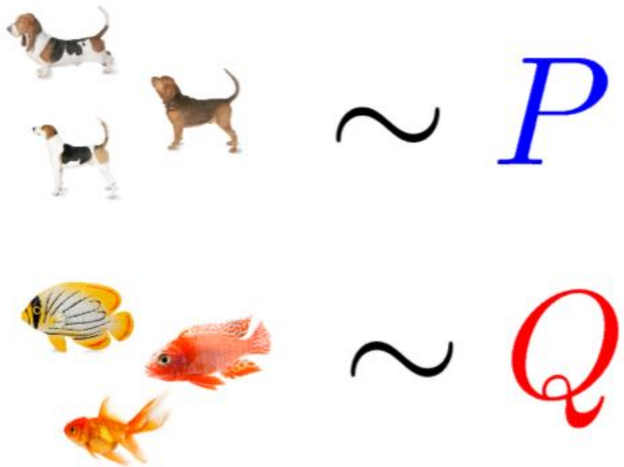

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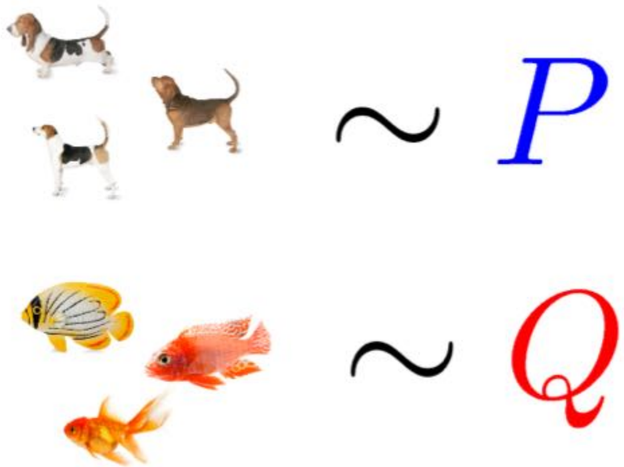

MMD slides courtesy of Wittawat Jitkrittum

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$$\mathrm{MMD}(p, q) := \left\| \mathbb{E}_{x \sim p}[\phi(x)] - \mathbb{E}_{y \sim q}[\phi(y)] \right\|_{\mathcal{H}},$$

where $\phi(x)$ is in the Hilbert space $\mathcal{H}$.

- Recall $\|a - b\|^2 = \langle a, a \rangle - 2 \langle a, b \rangle + \langle b, b \rangle$.

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Maximum Mean Discrepancy (MMD) [Gretton et al., 2012a]

- Define $k(x, x') := \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}$ (kernel).

$$\begin{aligned}\mathrm{MMD}_k^2(p, q) &= \left\| \mathbb{E}_{x \sim p}[\phi(x)] - \mathbb{E}_{y \sim q}[\phi(y)] \right\|_{\mathcal{H}}^2 \\ &= \mathbb{E}_{x \sim p}\mathbb{E}_{x' \sim p} k(x, x') - 2\mathbb{E}_{x \sim p}\mathbb{E}_{y \sim q} k(x, y') \\ &\quad + \mathbb{E}_{y \sim q}\mathbb{E}_{y' \sim q} k(y, y').\end{aligned}$$

- Unbiased estimator:

$$\widehat{\mathrm{MMD}}_k^2(\mathsf{X}, \mathsf{Y}) = \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i} k(x_i, x_j) - \frac{2}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} k(x_i, y_j) + \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i} k(y_i, y_j).$$

- $k(x, x') \approx$ similarity between x and x'.

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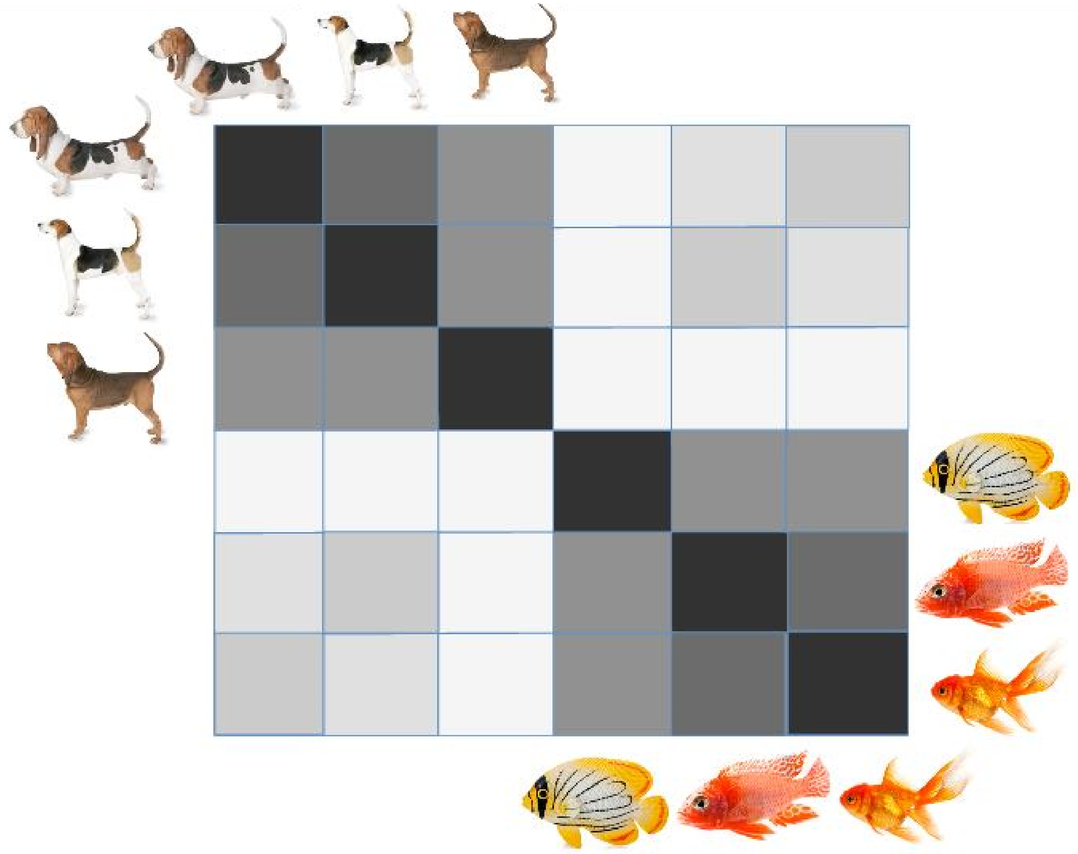
See Gretton et al. 2012 for the biased estimator

Intuition for the MMD

- Dogs $\sim p$ and fish $\sim q$.
- Each entry is one of $k(\text{dog}_i, \text{dog}_j)$, $k(\text{dog}_i, \text{fish}_j)$, or $k(\text{fish}_i, \text{fish}_j)$



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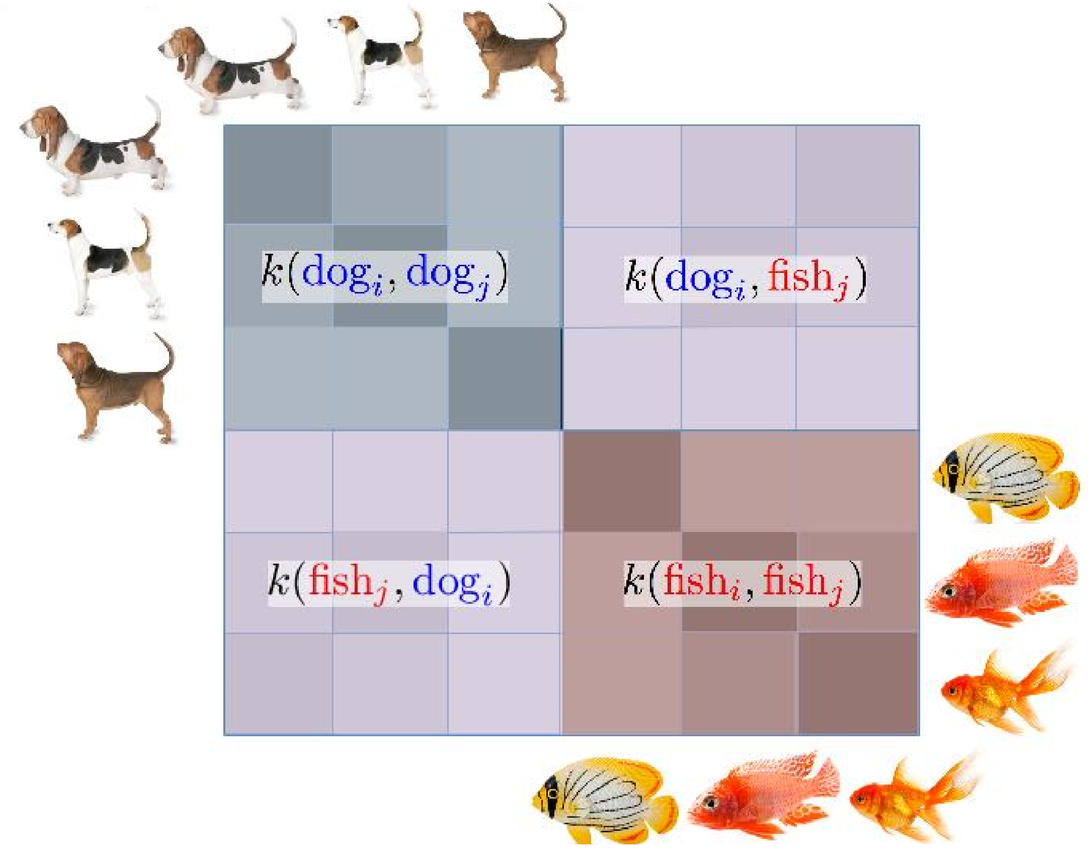
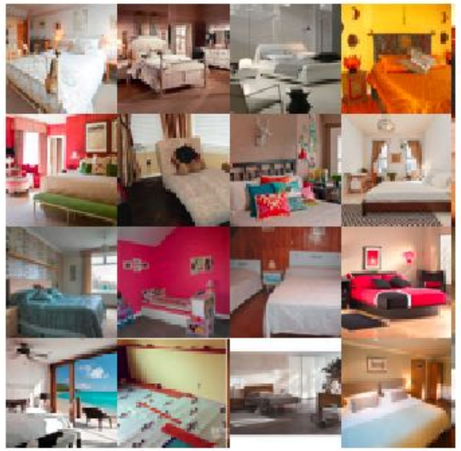
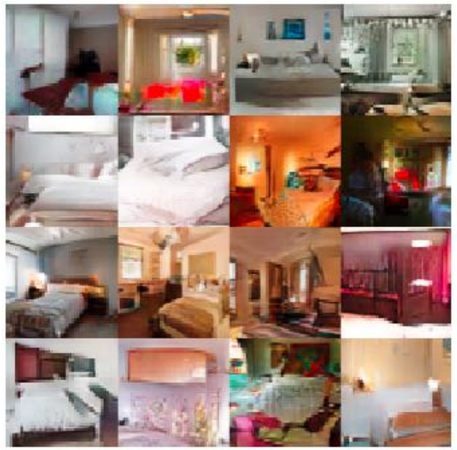
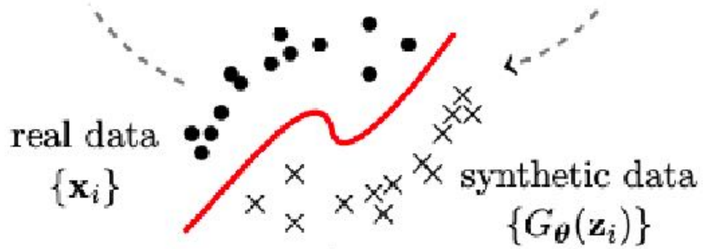


Application to generative modeling: MMD for generative adversarial nets (GAN)







MMD Test

$\left\| \hat{\mu}_X - \hat{\mu}_{G_{\boldsymbol{\theta}}(Z)} \right\|_{\mathscr{H}}$ is zero?

Comparison: Wasserstein-1 vs. MMD-k

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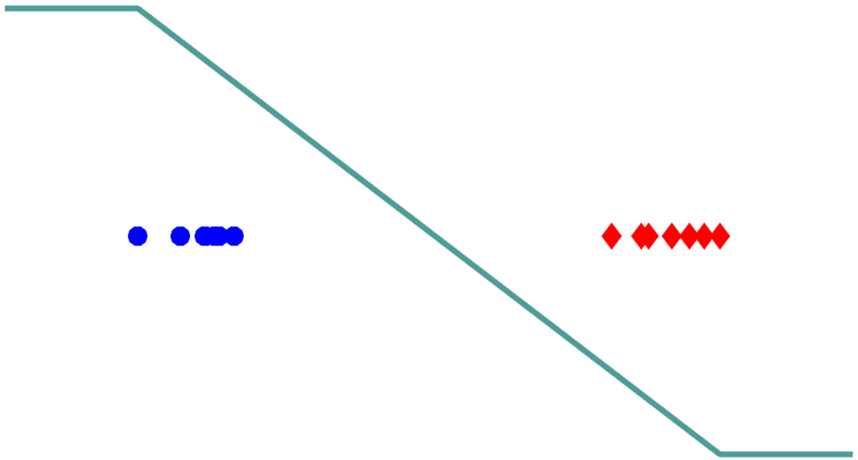
$W_1(P, Q) = \sup_{||f||_L \leq 1} E_P f(X) - E_Q f(Y).$

$||f||_L := \sup_{x \neq y} |f(x) - f(y)| / ||x - y||$

W_1=0.88



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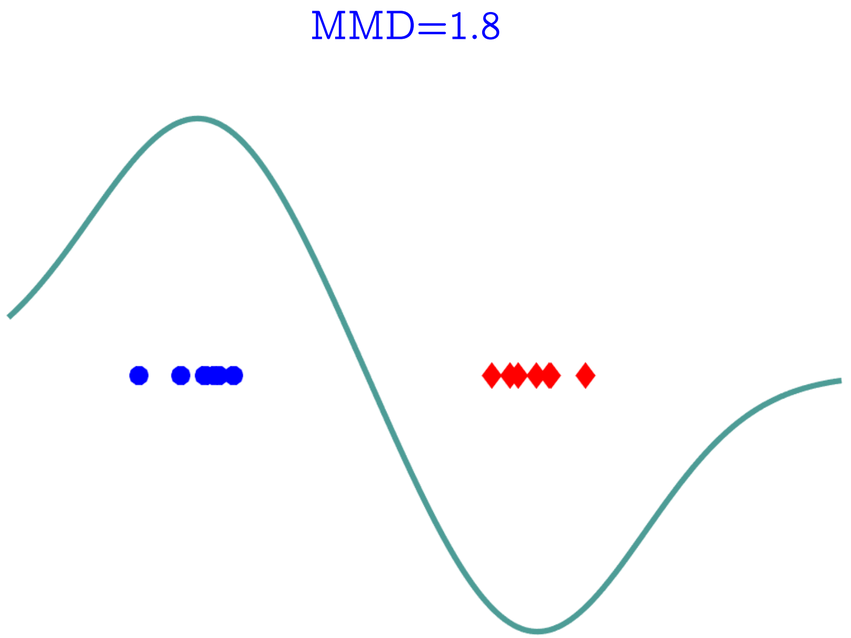

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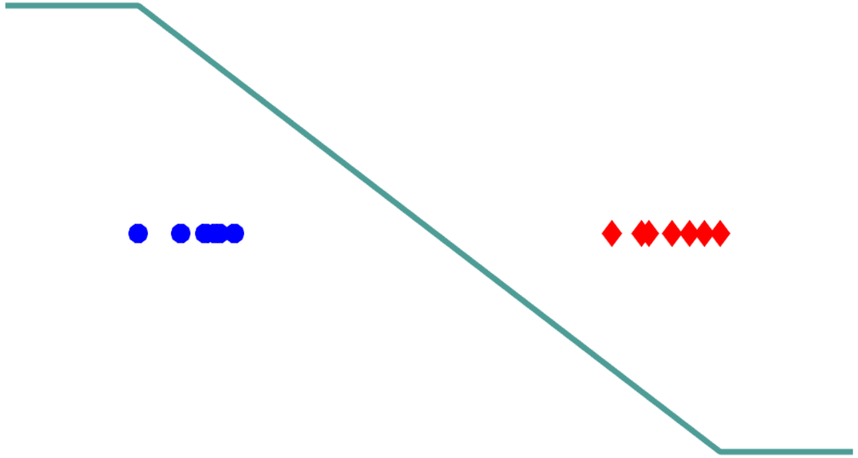

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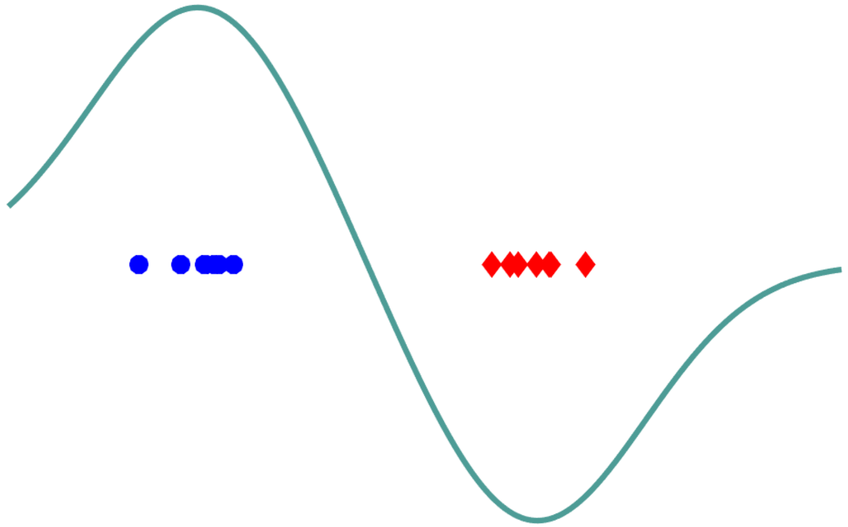

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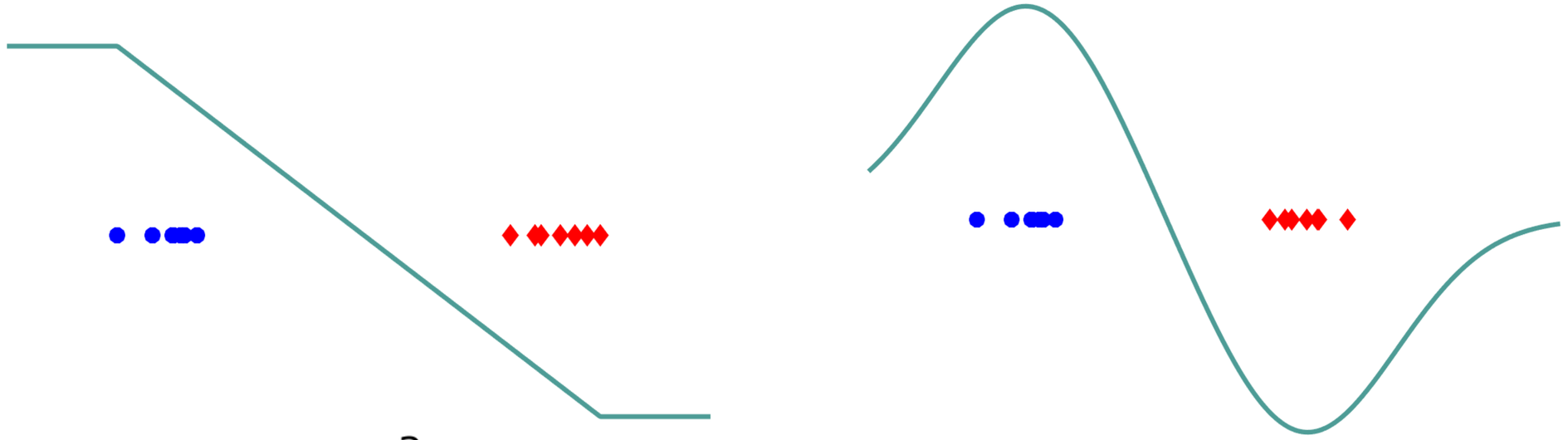

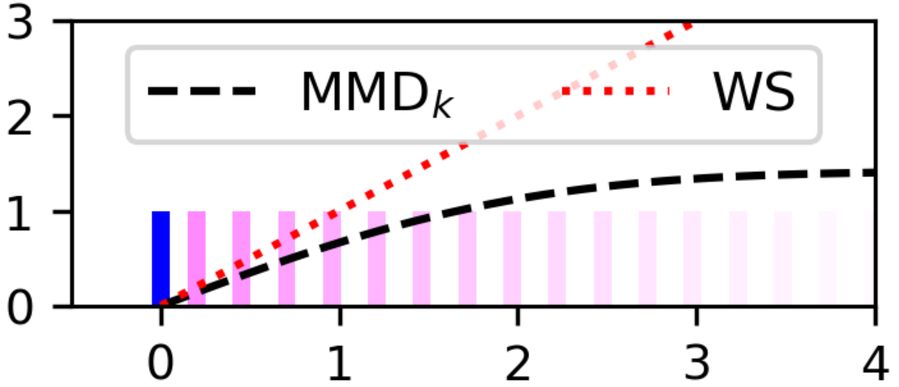

Distributional Robustness

Combine the strengths of ERM and RO: distributionally robust optimization (DRO)

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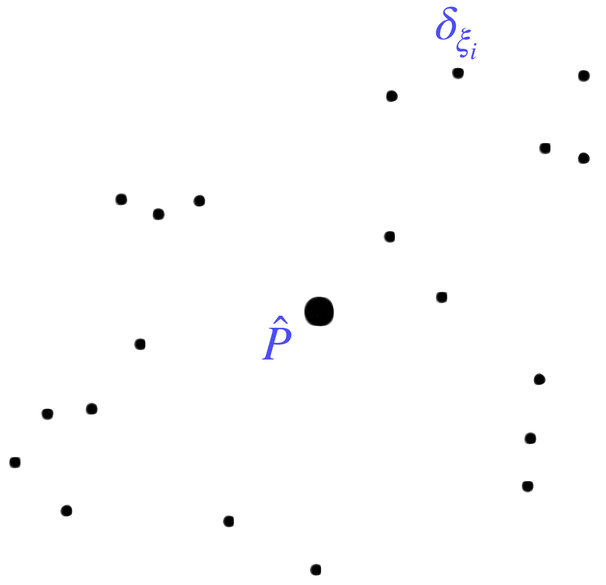

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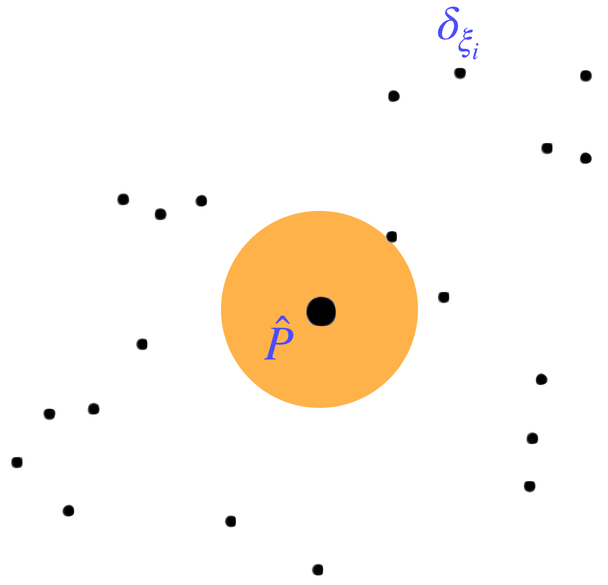

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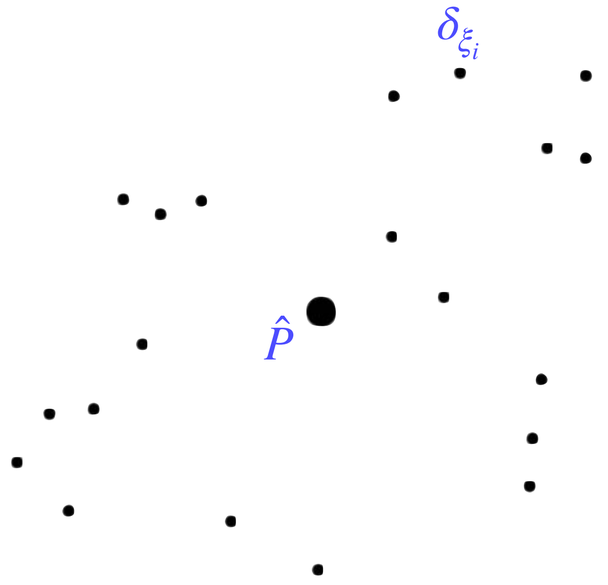

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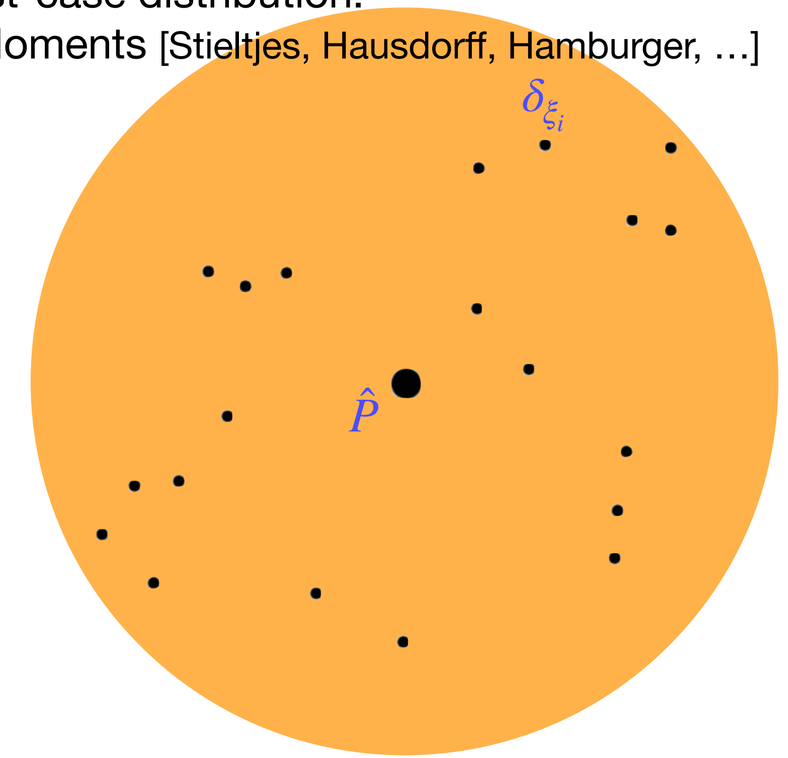

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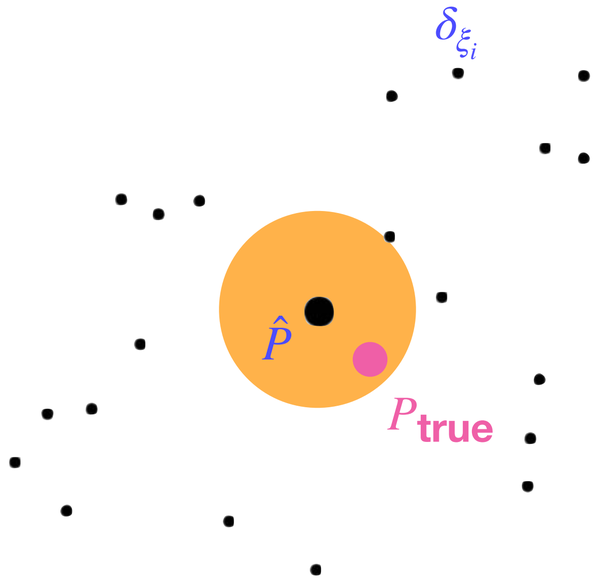
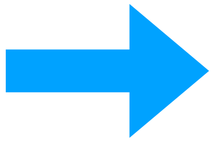
    - One way of constructing ambiguity region: one can quantify the empirical mean convergence rate $\gamma(\hat{P}, P_{\text{true}}) \leq \epsilon$.



What distributions does the ambiguity set $\mathscr{K}$ contain?

$$\min_{\theta} \sup_{\xi \in \mathscr{X}} l(\theta, \xi) \quad \text{(RO)}$$

Uncertainty set



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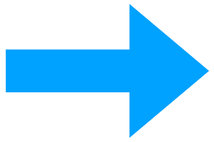

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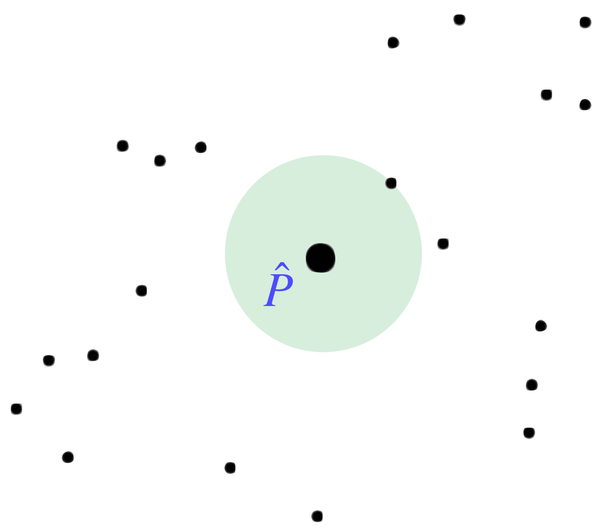

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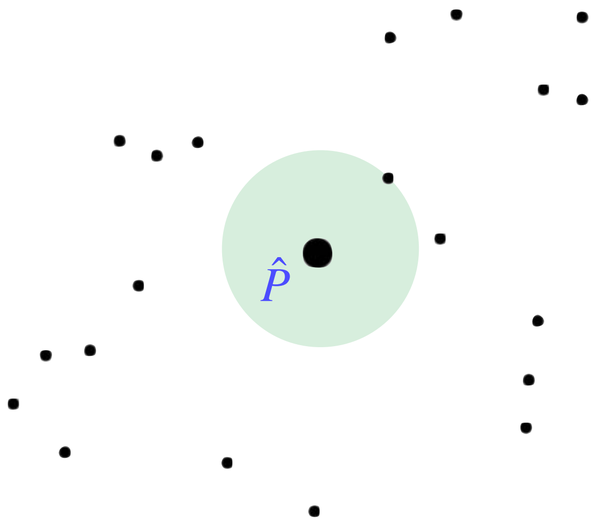

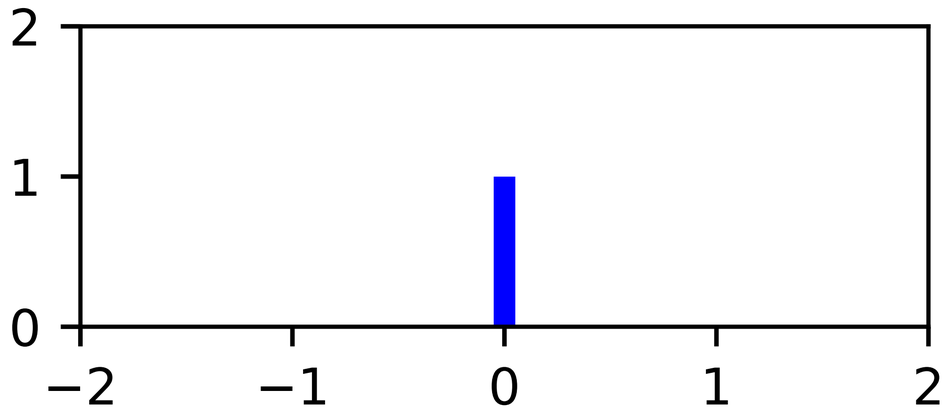

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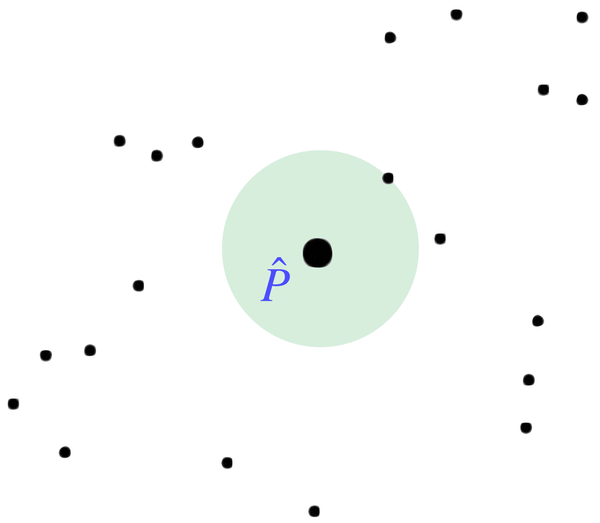

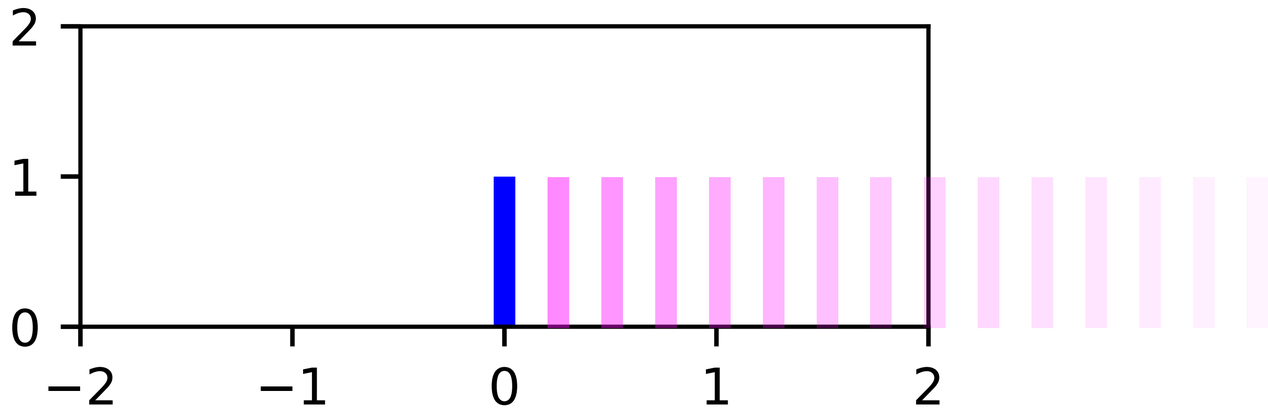

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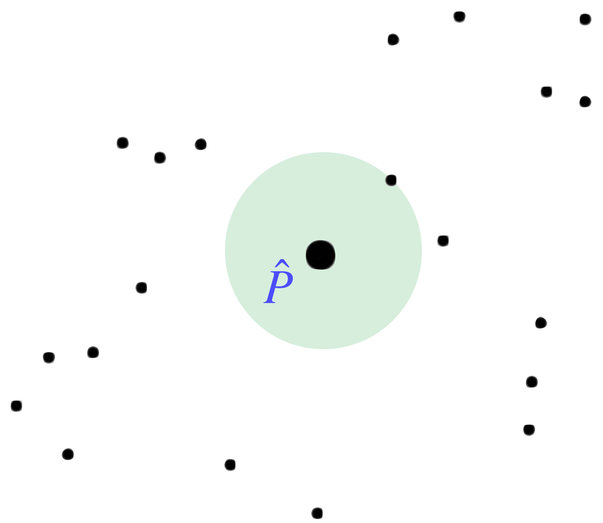

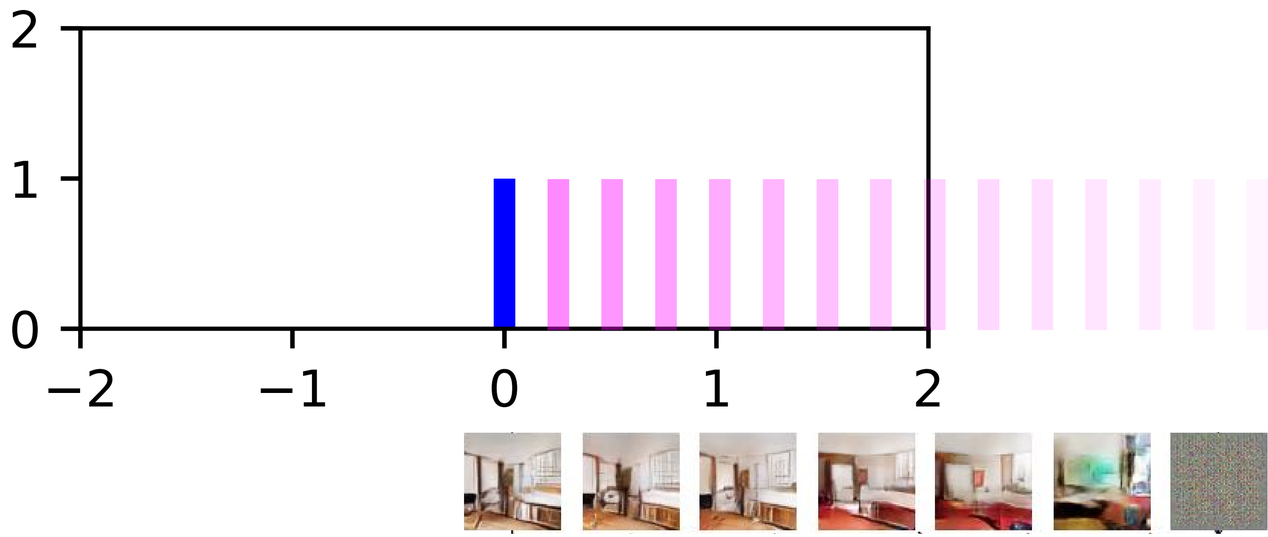

Image credit: Arjovsky'17

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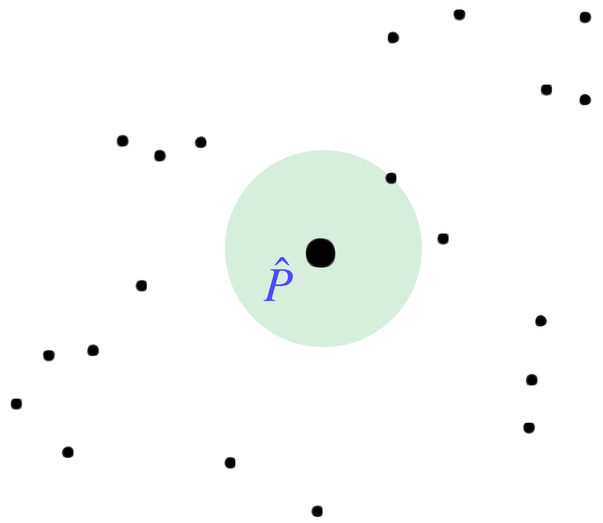

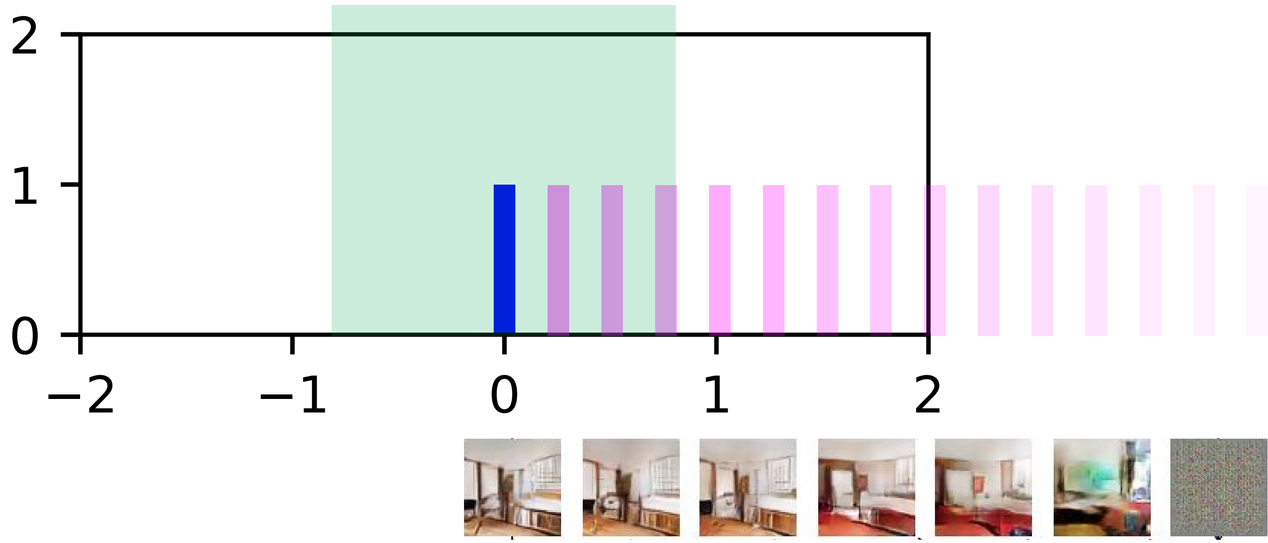

Image credit: Arjovsky'17

What distributions does the ambiguity set $\mathscr{K}$ contain?

$$\min_{\theta} \sup_{\xi \in \mathscr{X}} l(\theta, \xi) \quad \text{(RO)}$$

Uncertainty set

$$\min_{\theta} \sup_{P \in \mathscr{K}} \mathbb{E}_P l(\theta, \xi) \quad \text{(DRO)}$$

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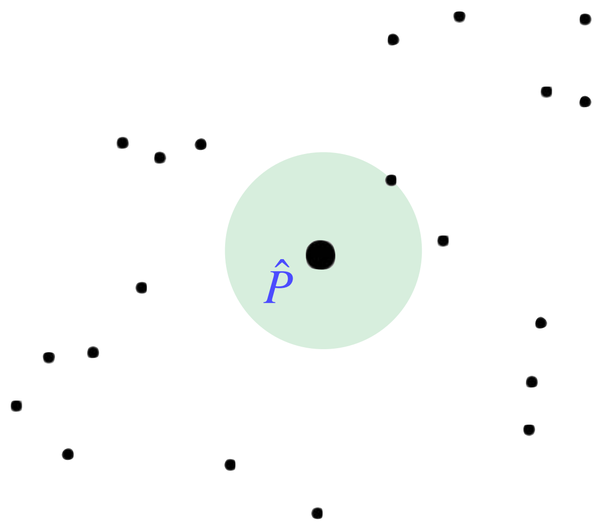

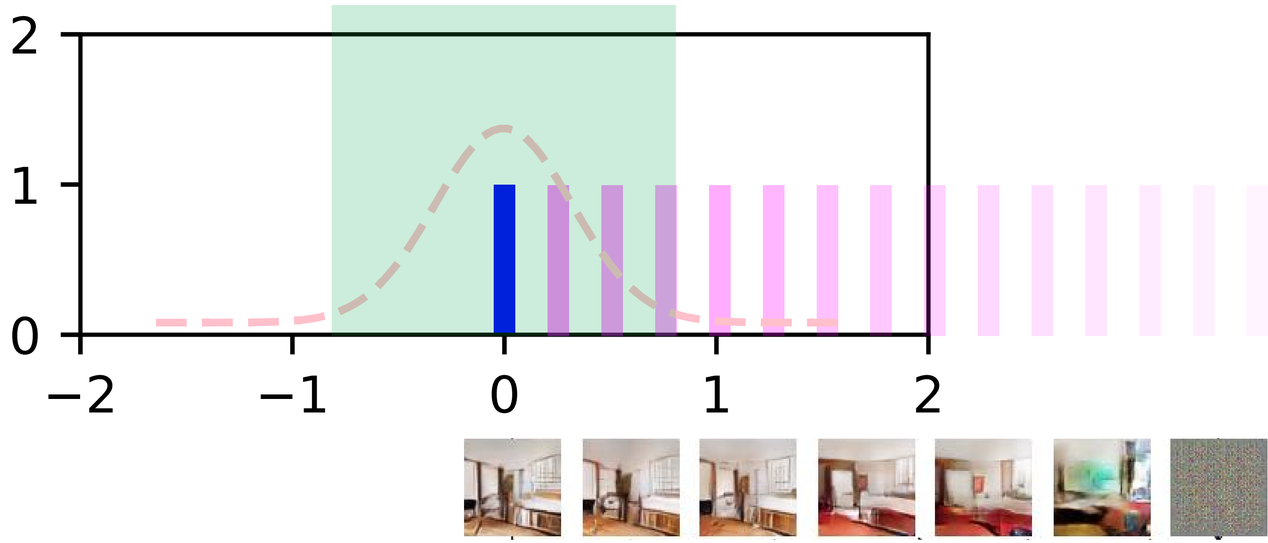

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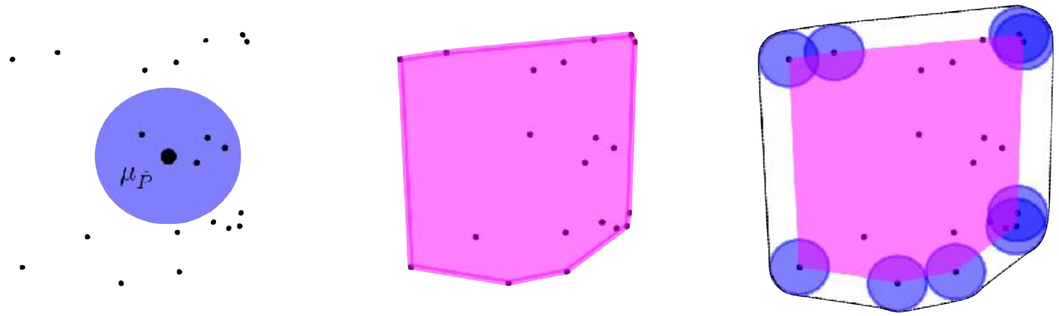

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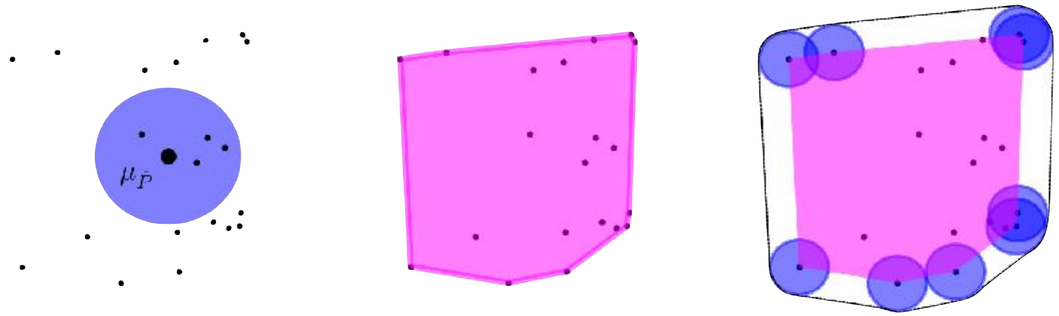

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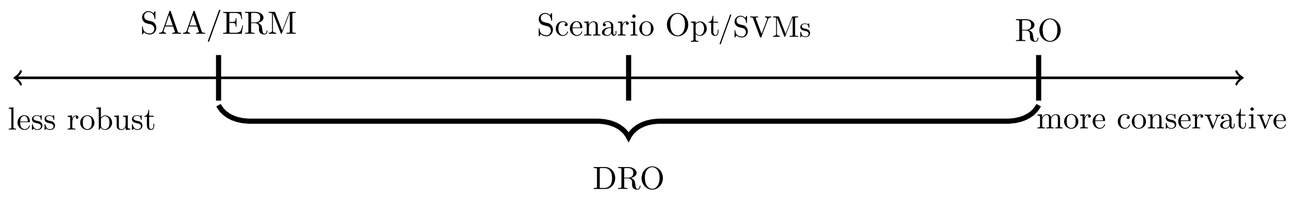

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- By comparing them, we find that DRO has the same structure as RO! This motivates us to solve DRO with convex duality (but DRO is ∞ -dimensional!).

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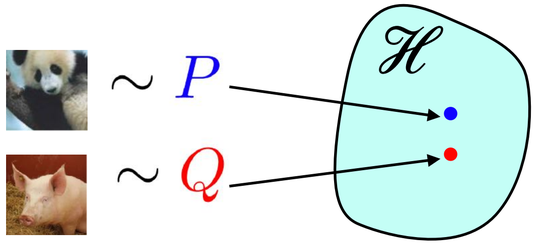

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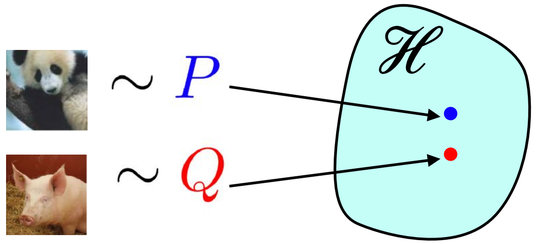

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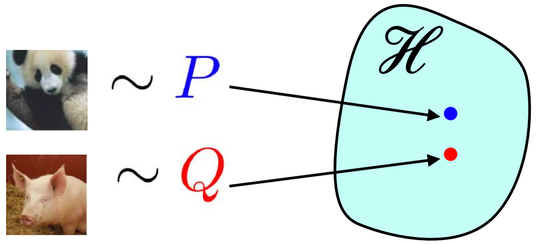

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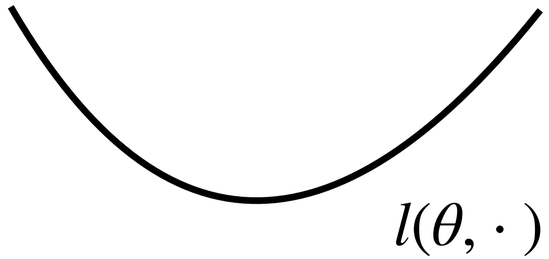

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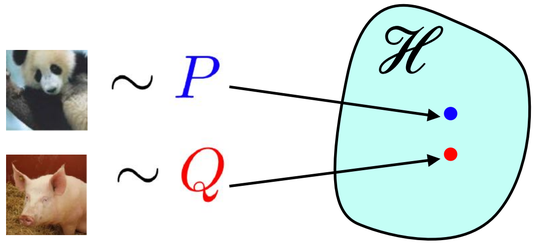

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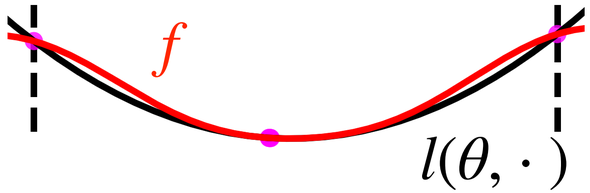

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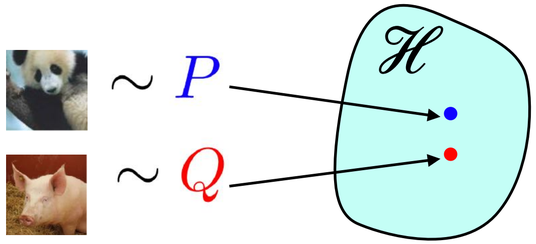

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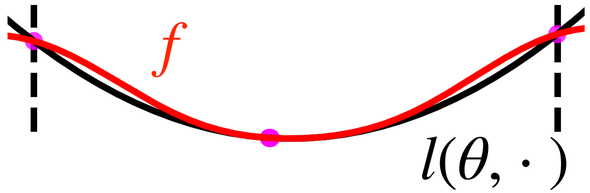

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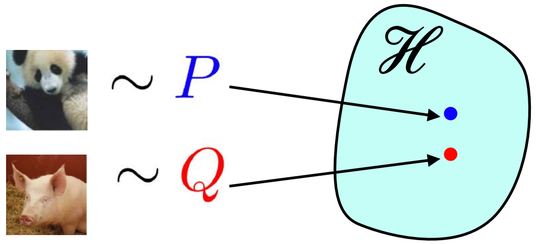

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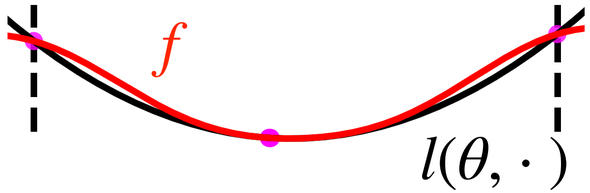

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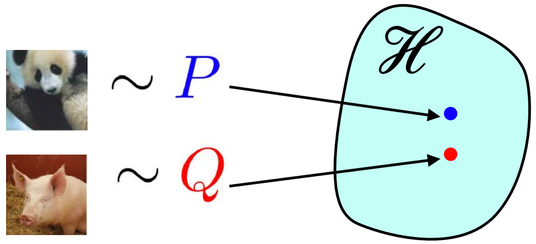

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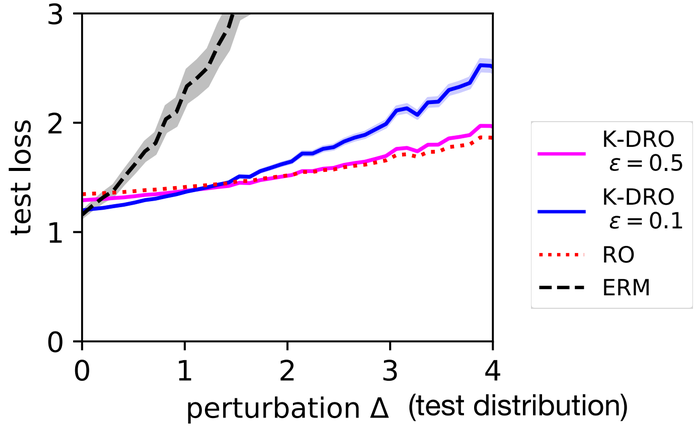

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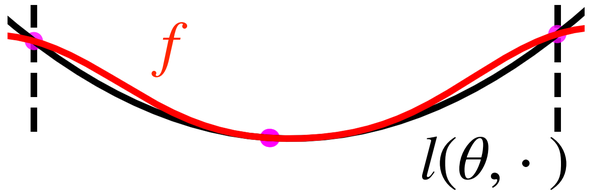

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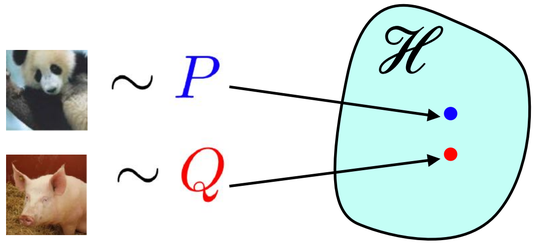

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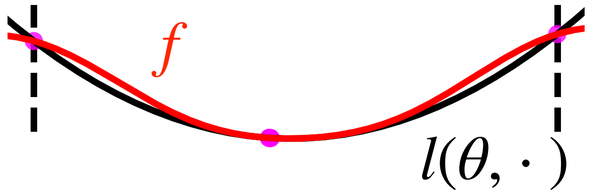

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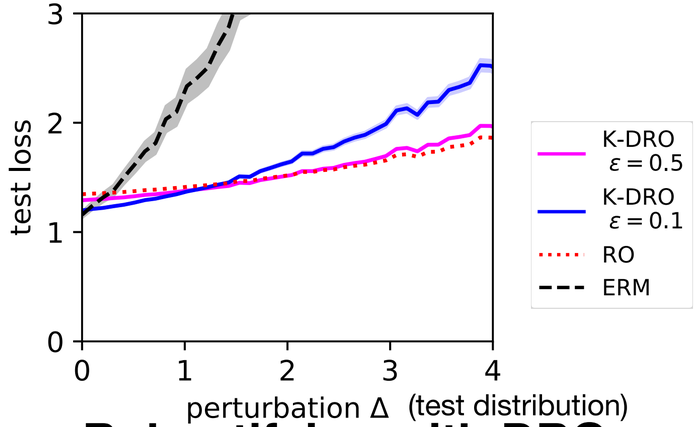

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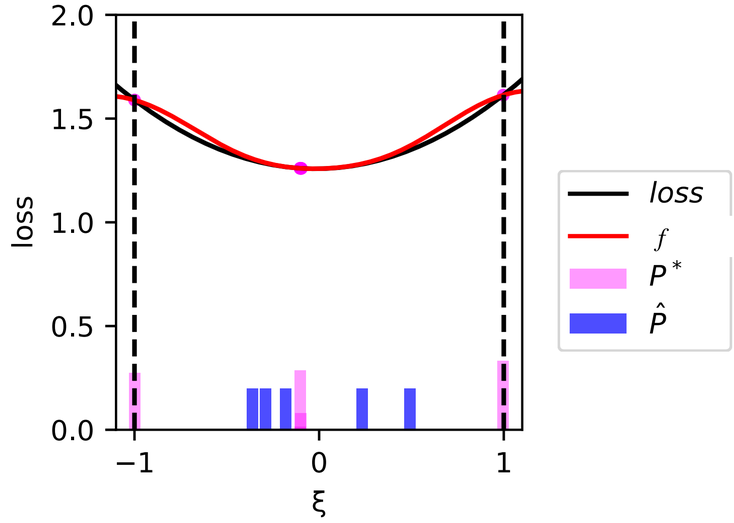

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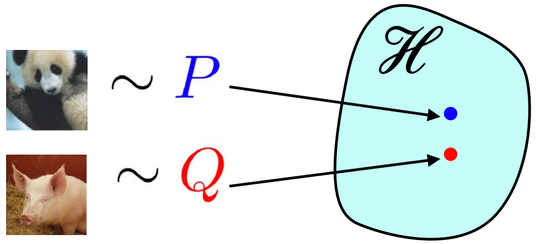

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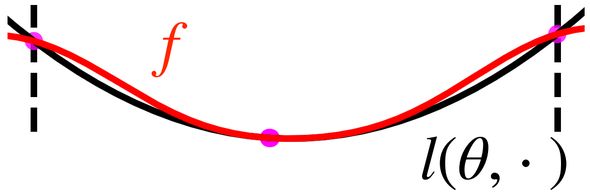

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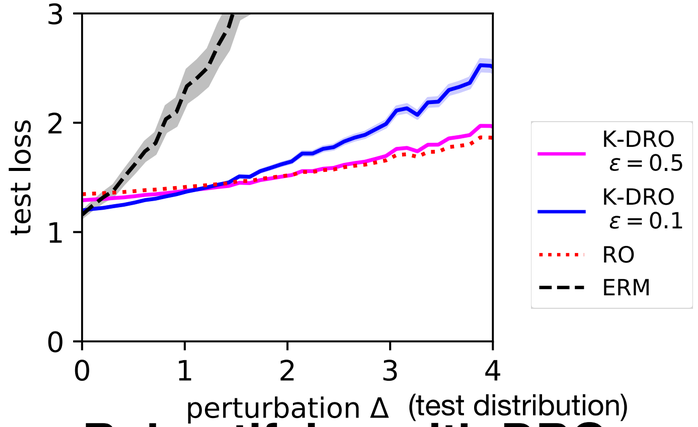

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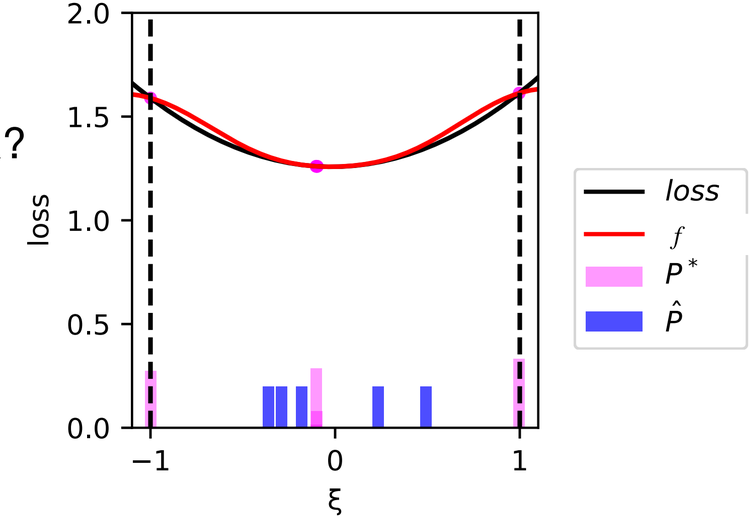

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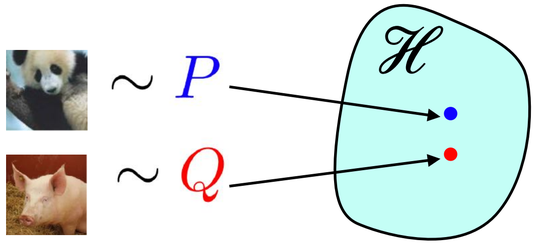

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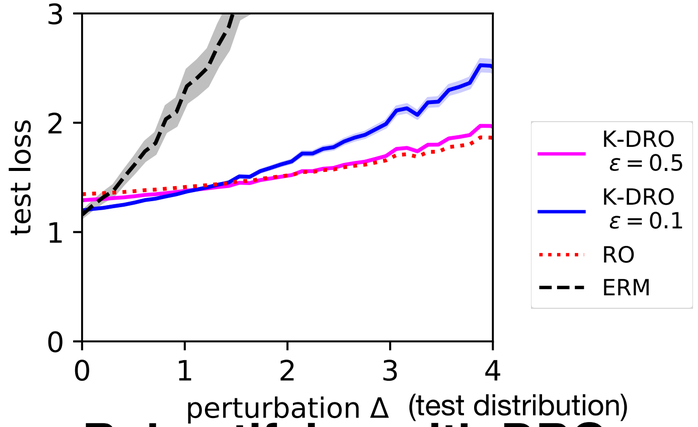

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Robustifying with DRO

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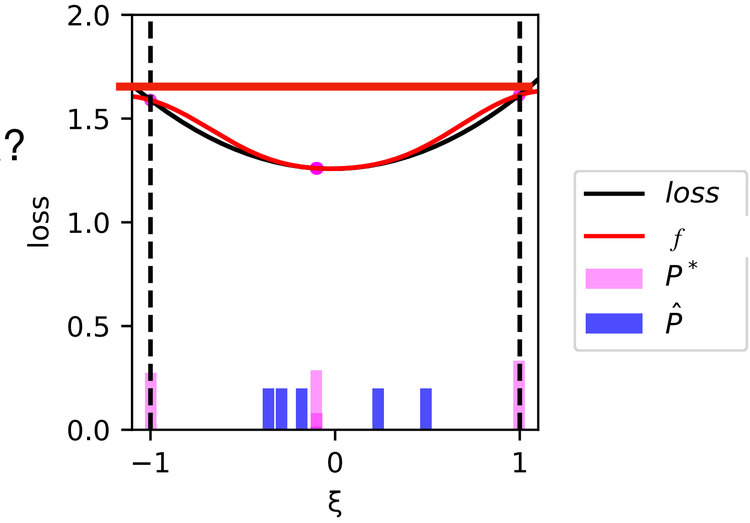
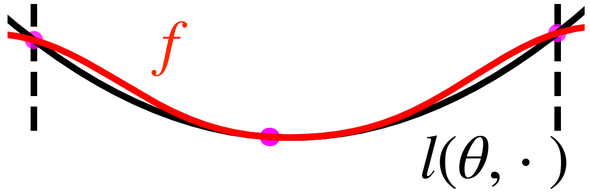


Geometric intuition



Smoothness of f ↔ Distributional robustness (↔ Size of $\mathscr{H}$)

Intuition: **flatten the curve, smooth is robust**

Special cases of DRO dual program

$$\text{(P)}\ \min_{\theta}\ \sup_{\gamma(P,\hat{P})\le\epsilon}\ \mathbb{E}_{P} l(\theta,\xi) \quad \Longleftrightarrow \quad \text{(D)}\ \min_{\theta, f\in\mathscr{H}}\ \mathbb{E}_{\hat{P}} f + \epsilon \|f\|_{\mathscr{H}} \quad \text{s.t.}\ l(\theta,\cdot) \le f$$

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- Type-1 Wasserstein DRO. Suppose the loss function $l(\theta,)$ is Lipschitz continuous, and we choose γ to be the W-1 distance. (D) is then equivalent to Lipschitz regularized ERM

$$\min_{\theta}\frac{1}{N}\sum_{i=1}^{N} l(\theta,\xi) + \epsilon\mathrm{Lip}(l).$$

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- Kernel DRO. If we choose to be the MMD, then solving DRO becomes a kernel-based learning

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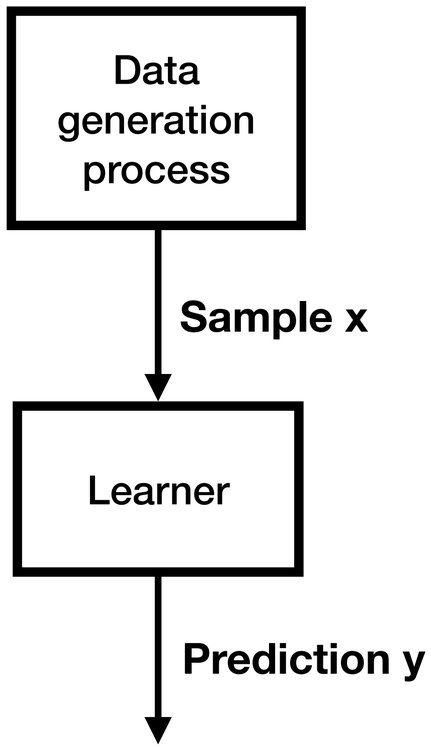
Multi-stage robust decision-making

SL



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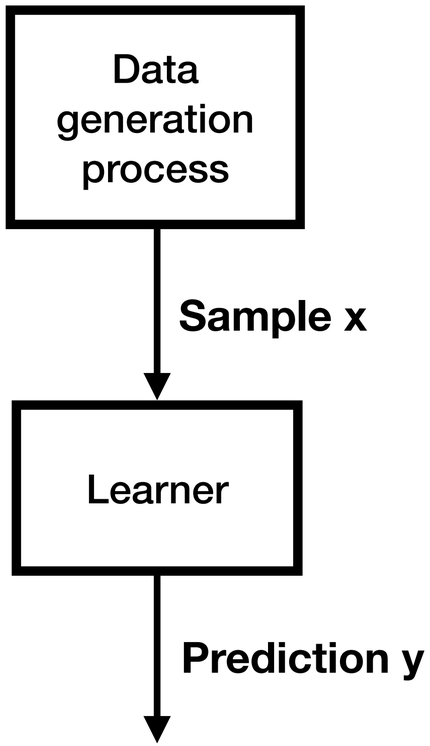
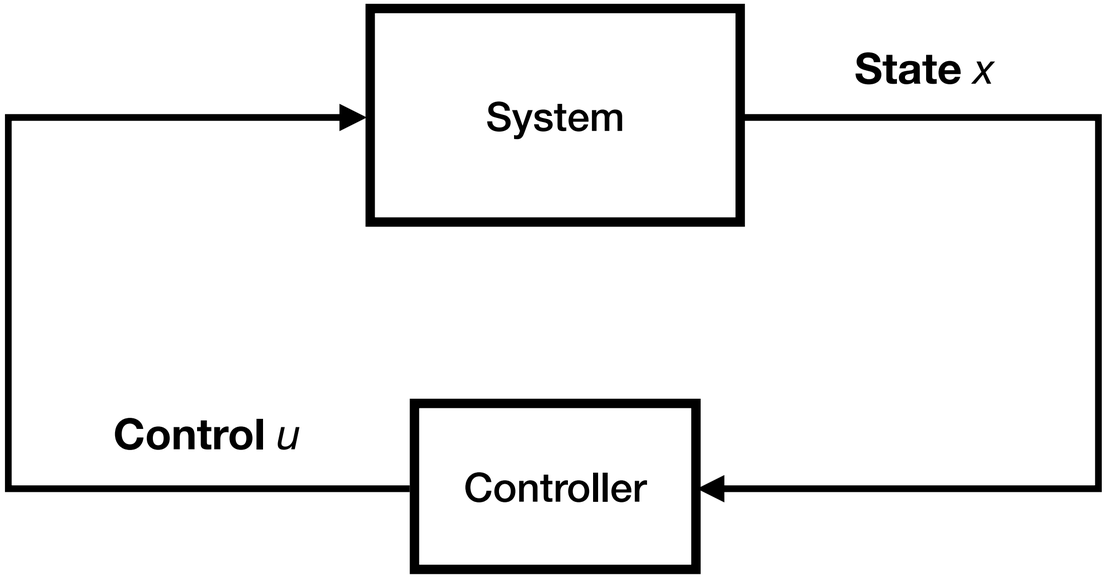
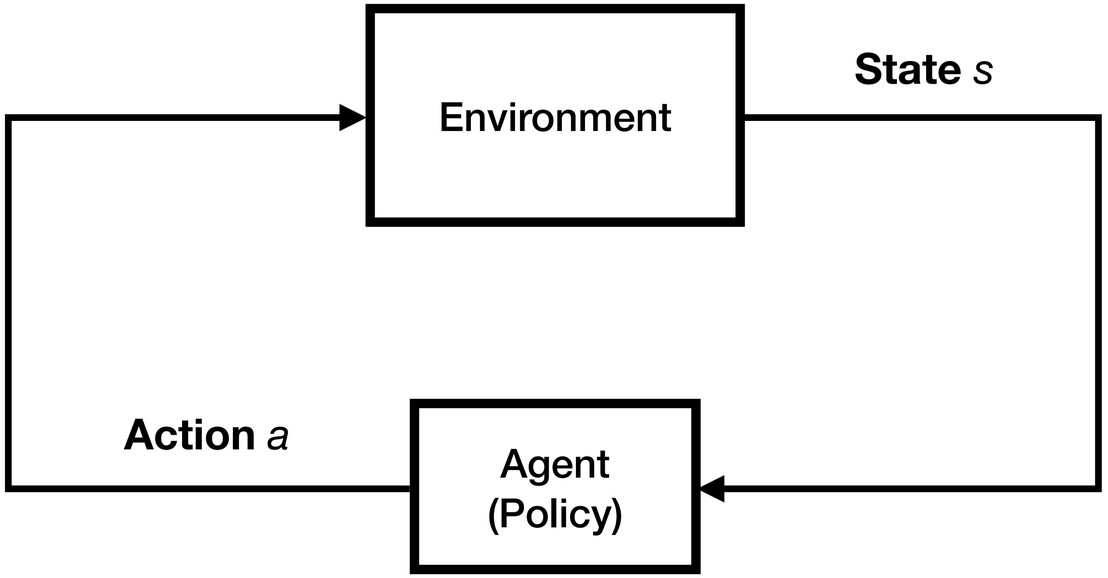


Control

RL





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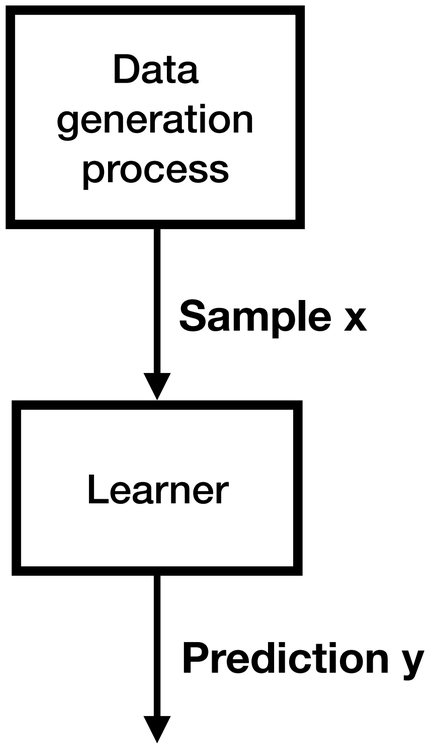

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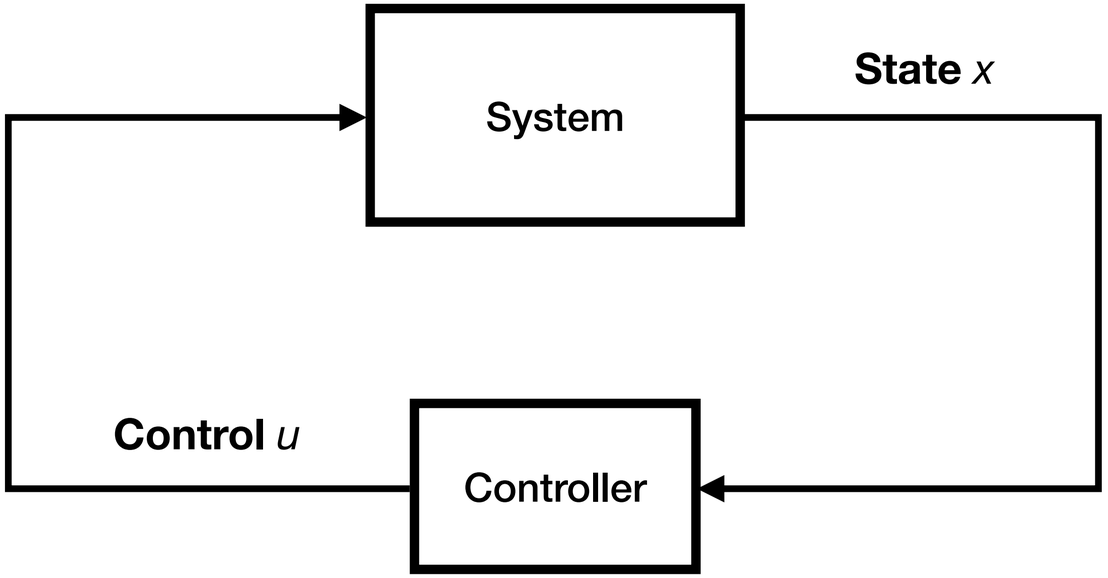

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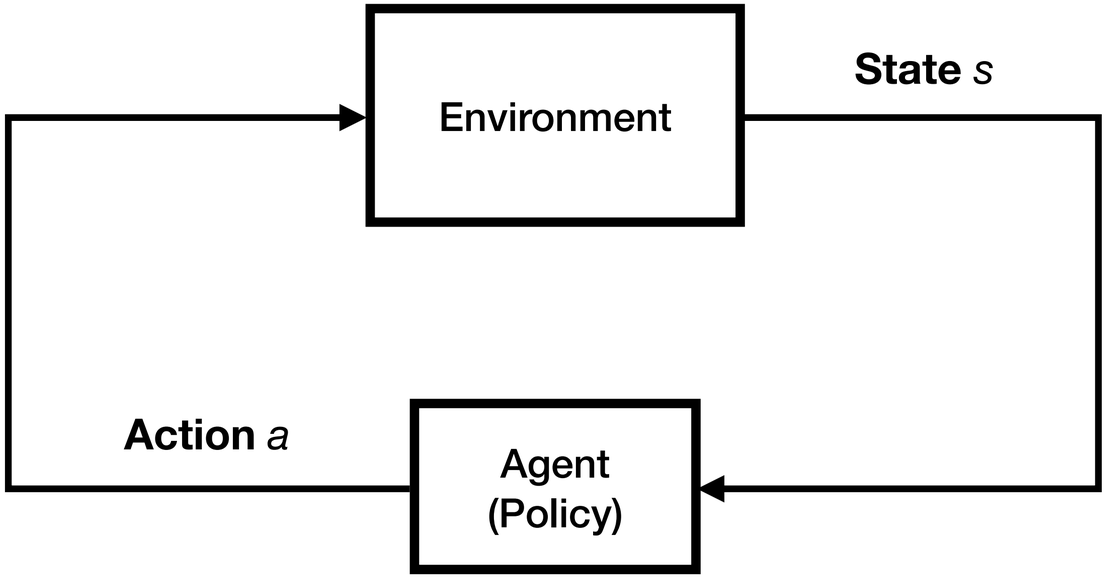

Distinction: feedback in systems causes **distribution shift** in the data-generation processes

Reinforcement learning problem

$$\max_{\mu} \quad \mathbb{E} \sum_{t=1}^{T} \textbf{reward}(x_t, \mu(x_t))$$

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Optimal control problem

Why do we need to be robust in RL/control?

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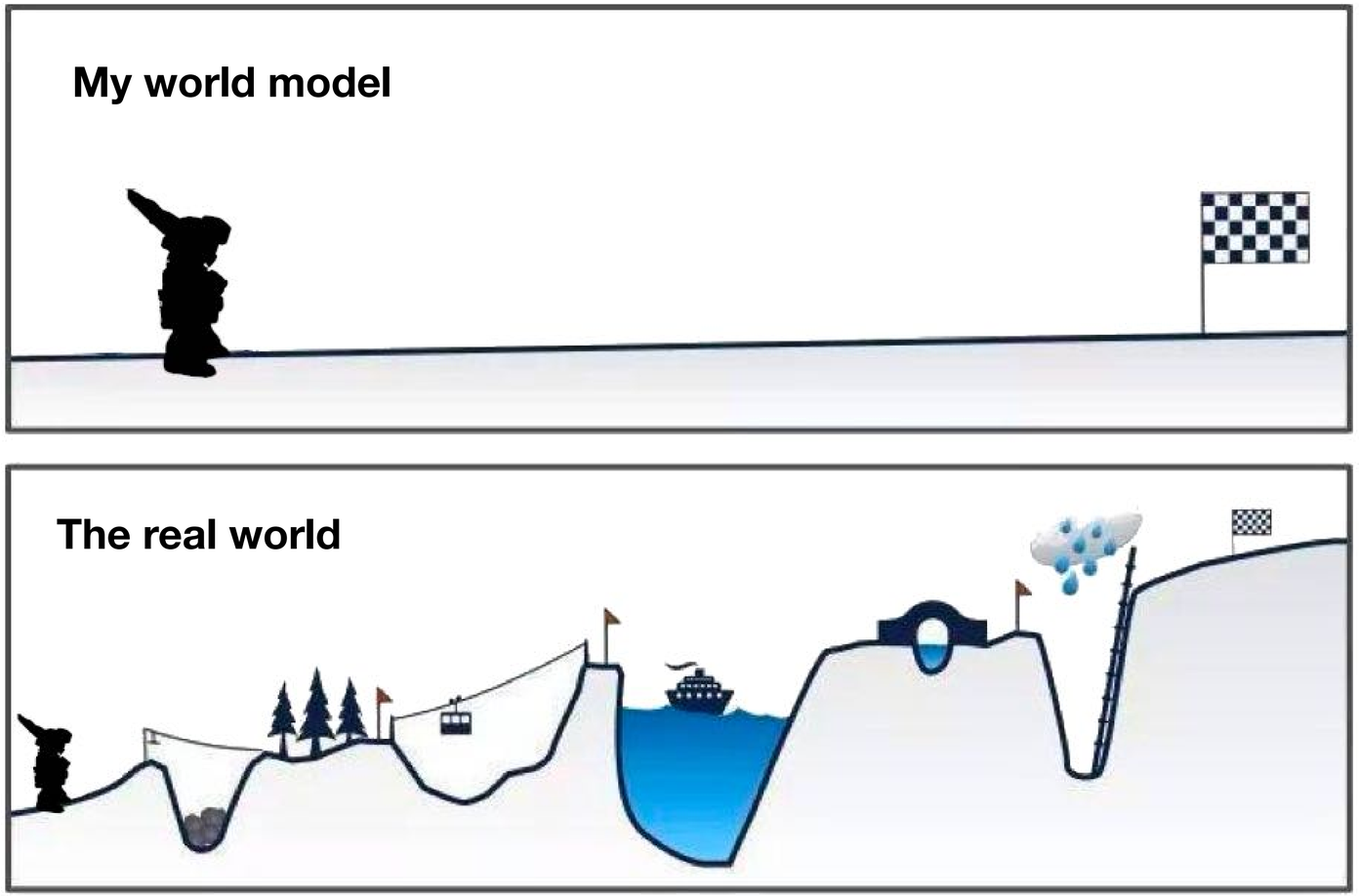

Model Predictive Control

Model Predictive Control

Optimal control problem

(discrete-time)

$$\underset{u_0,\ldots,u_{N-1}}{\text{minimize}} \quad \sum_{t=1}^{N-1} l_t(x_t, u_t) + l_N(x_N)$$

$$\text{subject to} \quad x_{t+1} = f(x_t, u_t)$$

$$c(x_t, u_t) \leq 0$$

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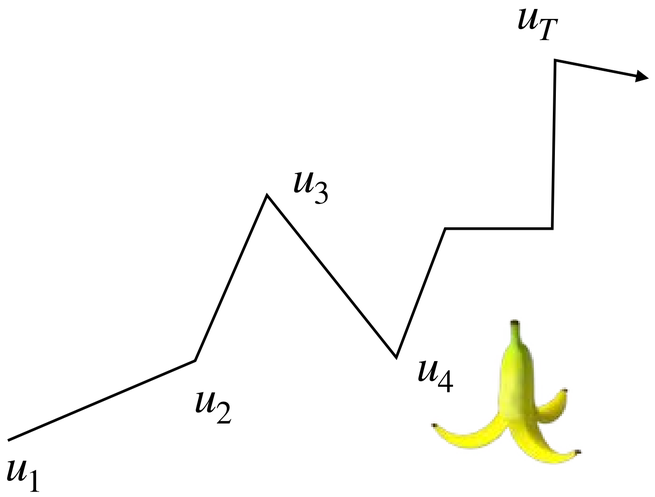

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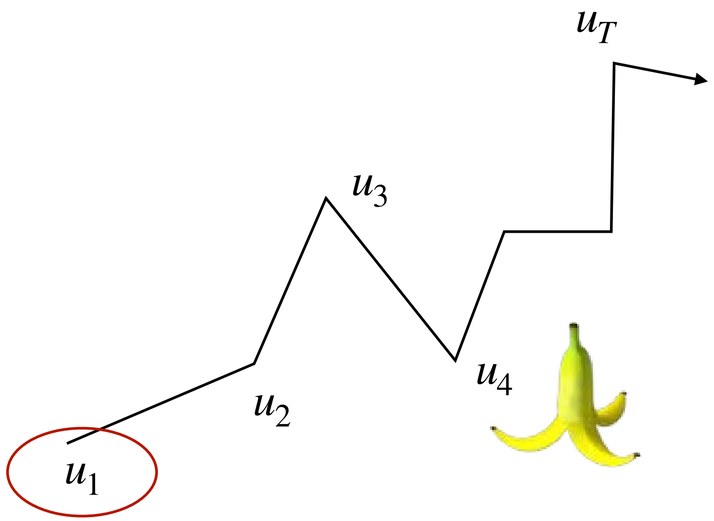

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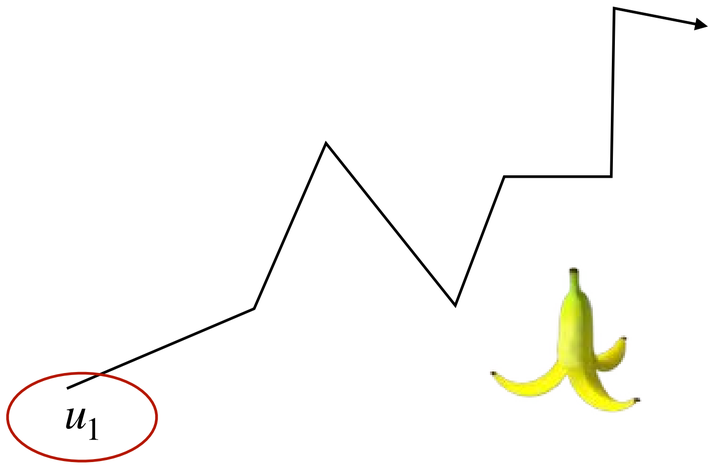

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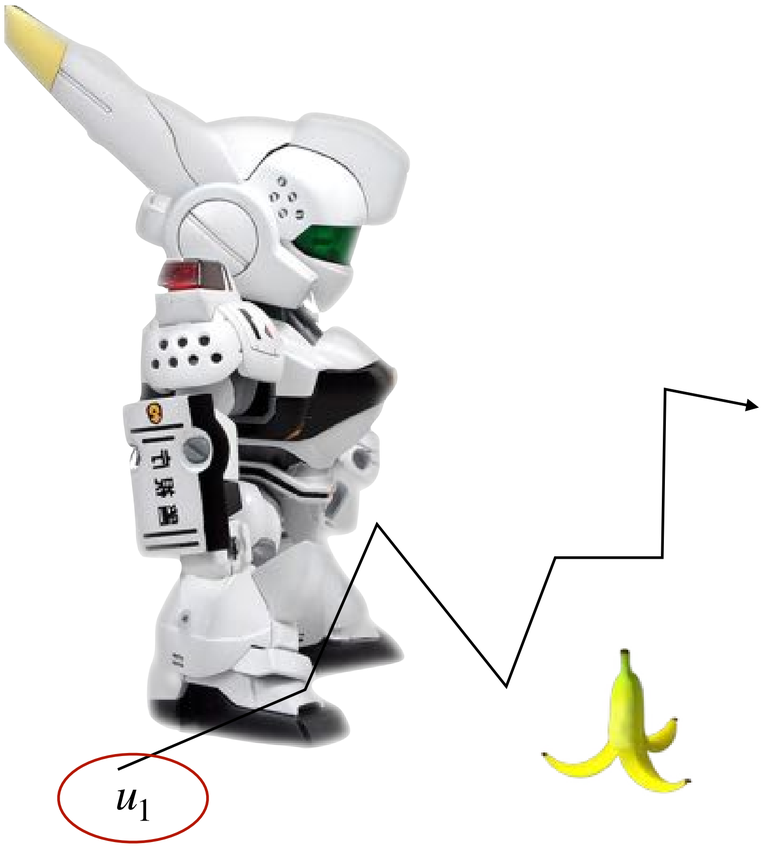

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You are using MPC when you drive or catch a train.

Learning-based MPC is an active research area!

Robust and stochastic model predictive control

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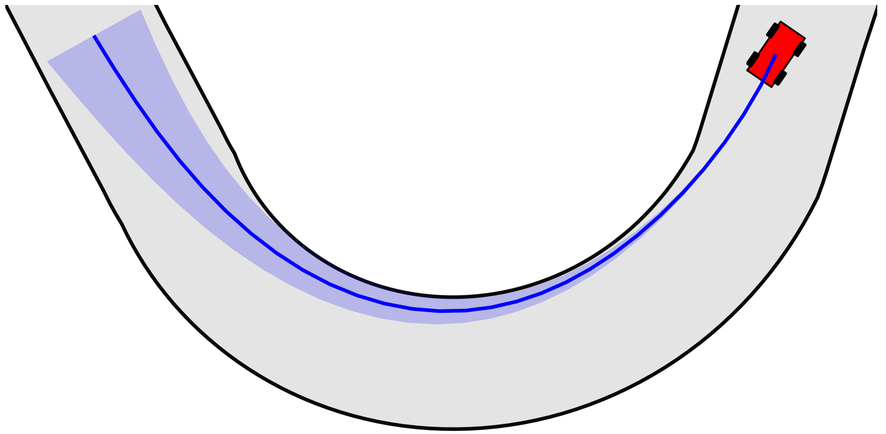

Figure credit: Hewing et al.'18, Z. et al.'20

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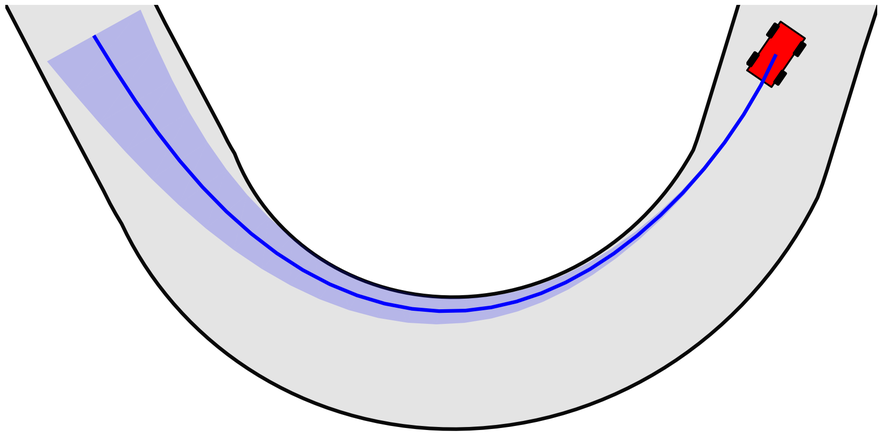

Guaranteed Margins for LQG Regulators

JOHN C. DOYLE

***Abstract*—There are none.**

Figure credit: Hewing et al.'18, Z. et al.'20

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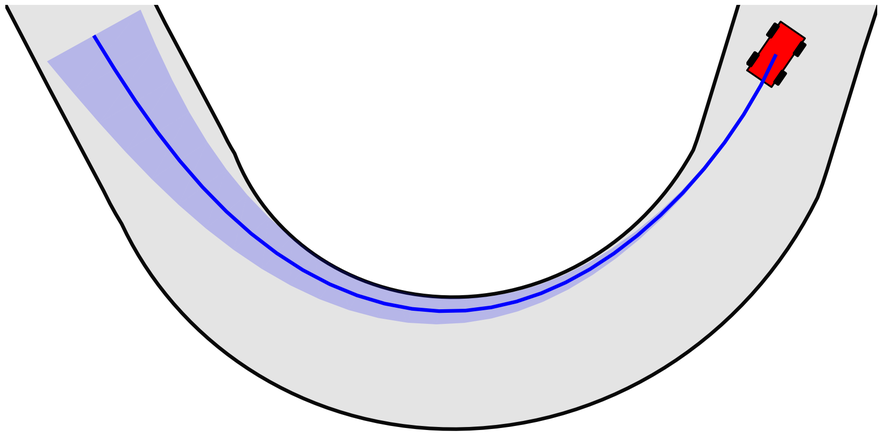

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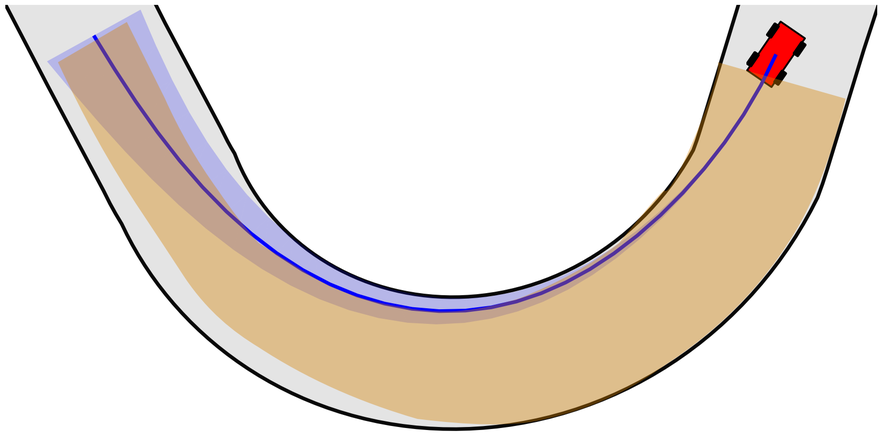

- **Constraint Tightening strategy**: Drive within a narrower "*tube*" than the original track!

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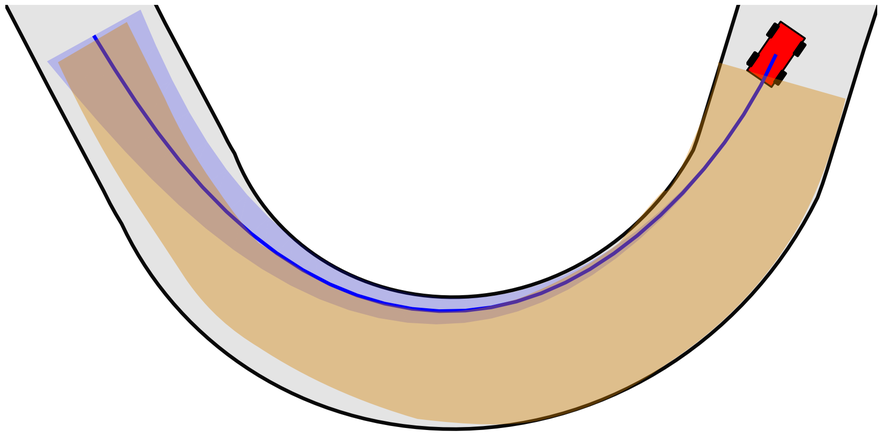

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Optimization (alone) is not robust.

- **Constraint Tightening strategy**: Drive within a narrower "*tube*" than the original track!
- In practice, this often boils down to replacing the constraint $c(x_t, u_t) \leq 0$ by

  $c(x_t, u_t) + b \leq 0$ for some $b > 0$.

Figure credit: Hewing et al.'18, Z. et al.'20

Learning for control:
Three main classes of methods

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They all suffer from distribution shift!

Covariate shift in imitation learning

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Train

Formula1Net π_θ

Covariate shift in imitation learning

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(IL): $\min_{\theta \in \Theta} \int \|\pi_\theta(x) - \pi_e(x)\|^2 \mu^{\pi_e}(dx),$

Covariate shift in imitation learning

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Covariate shift in imitation learning

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  But π_θ, π_e are only similar under the μ^{π_e}.

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- **Same goes for learning dynamics for control**

Fix: covariate shift in imitation learning

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DAgger (Data Aggregation)
1. Train a policy π_θ from expert data D
2. Run π_θ (on the robot) to obtain new states
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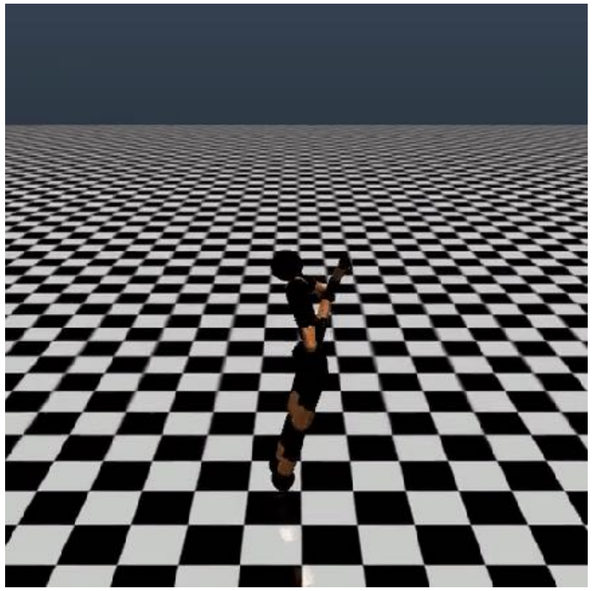
Fix: covariate shift in imitation learning



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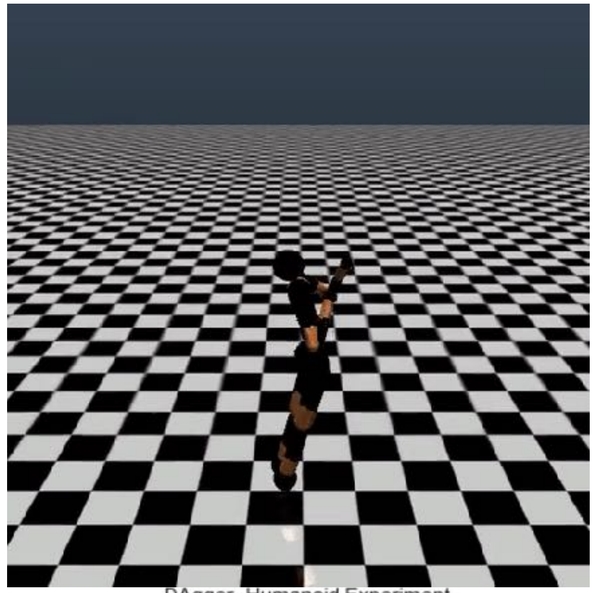

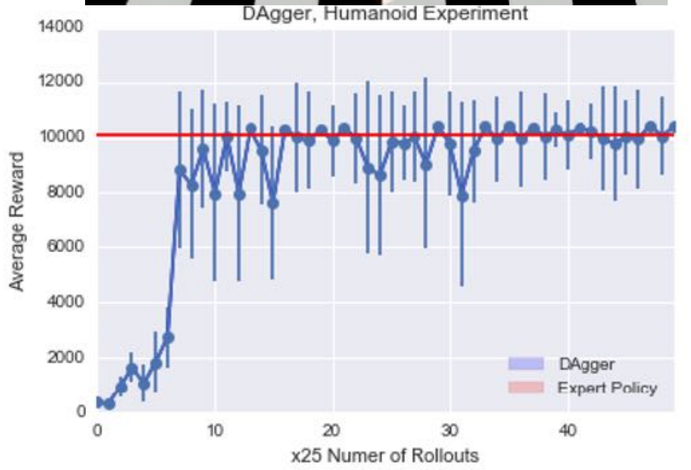

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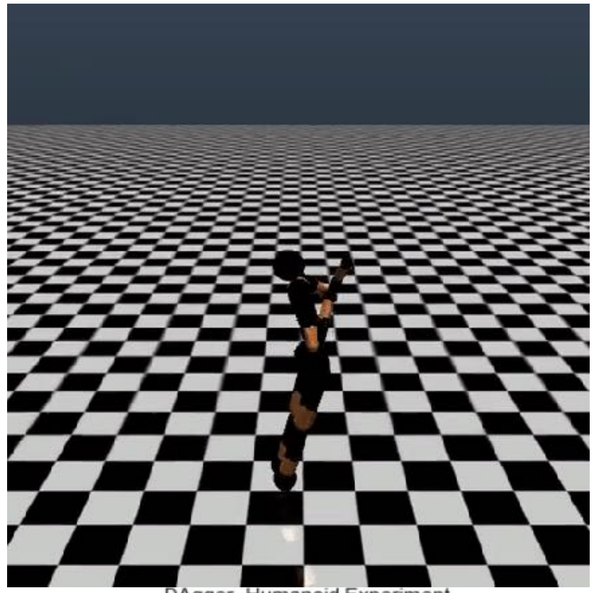

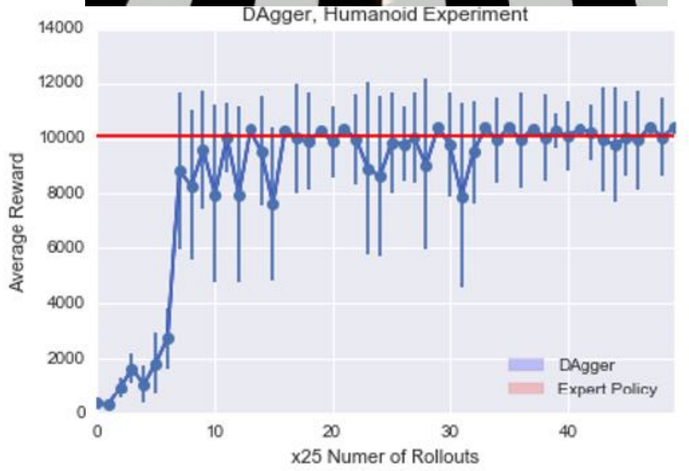

Other related topics: off-policy/offline RL

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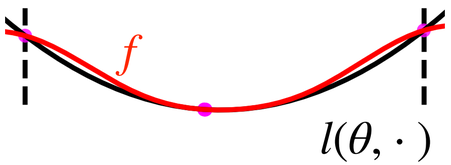

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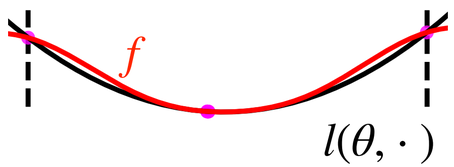

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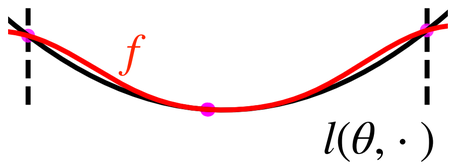

Other topics

- Generalizaiton and statistical bounds of DRO, minimax rate of non-parametric statistics
- Distributionally robust MPC
- Distributionally robust dynamics learning
- Off-policy RL, off-line RL
- Multi-stage DRO
- Adversarial attacks
- Causal inference
- Double descent
- Robust generative modeling
- You tell me!

Thank you!

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Max-Planck-Institute, Tübingen
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