Iterative Sampling Methods for Solving Sinkhorn Distributionally Robust Optimization

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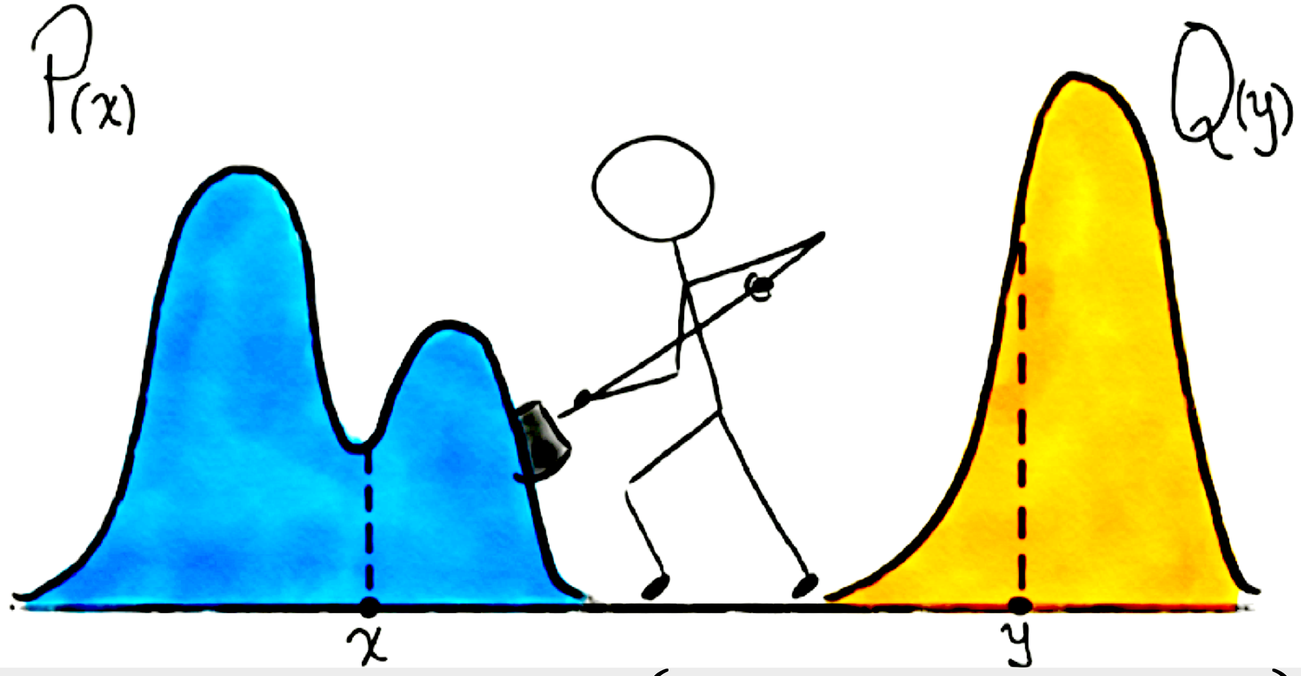
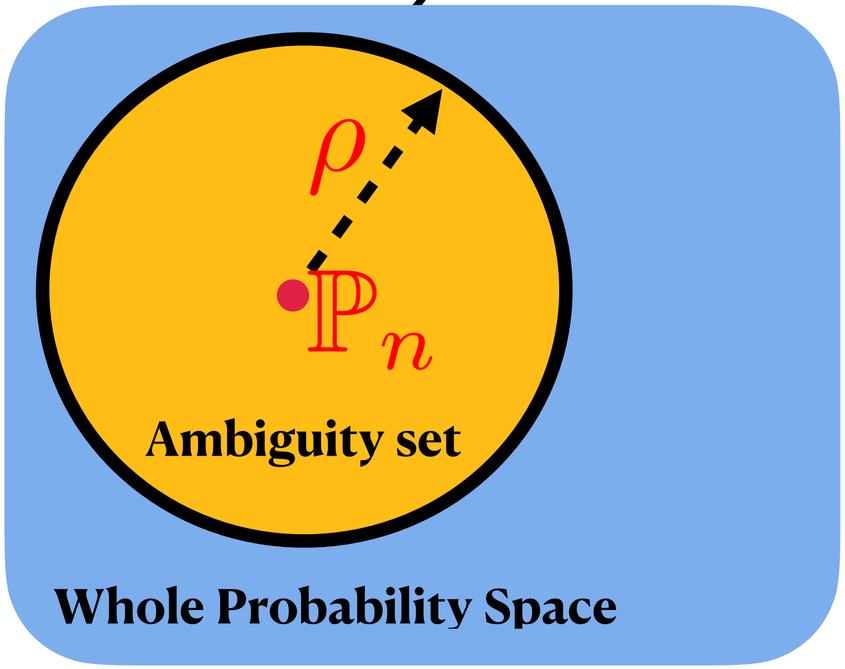
Wasserstein Distributionally Robust Optimization

$$\min_{\theta} \left\{ \sup_{\mathbb{P}:\ \mathcal{W}(\mathbb{P},\mathbb{P}_n)\leq\rho} \mathbb{E}_{z\sim\mathbb{P}}[\ell(z;\theta)] \right\}$$





$$\mathcal{W}(\mathbb{P},\mathbb{Q}) = \inf_{\gamma\in\Gamma(\mathbb{P},\mathbb{Q})} \left\{ \mathbb{E}_{(x,y)\sim\gamma}\left[\|x-y\|^2\right] \right\}_2$$

- data-driven, non-parametric, free of distributional assumptions

Tractability of Wasserstein DRO

$$\min_{\theta} \left\{ \sup_{\mathbb{P}:\ \mathcal{W}(\mathbb{P},\mathbb{P}_n)\le\rho} \mathbb{E}_{z\sim\mathbb{P}}[\ell(z;\theta)] \right\}$$

$$= \min_{\theta,\lambda\ge 0} \left\{ \lambda\rho + \mathbb{E}_{x\sim\mathbb{P}_n}\left[\underbrace{\sup_{z} \left\{ \ell(z;\theta) - \lambda\|x-z\|^2 \right\}}_{\text{Moreau-Yoshida regularization}} \right] \right\}$$ **(Strong Dual Reformulation)**

1. Probability support is *discrete* and *finite* [Pflug G et. al 2008, ...]
2. Loss $\ell(z;\theta)$ is *piecewise concave / generalized linear model* [Esfahani PM et. al 2018, Shafieezade et al 2015, ...]
3. $z \mapsto \ell(z;\theta) - \lambda^*\|x-z\|^2$ is *strongly concave* [Sinha et. al 2018, ...]

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Cons: Wasserstein DRO is not necessarily tractable for general applications

Literature Review on Infinite-Dimensional Optimization

$$\min_{\rho \in \mathscr{P}(\mathbb{R}^d)} \quad \mathscr{F}(\rho)$$

1. Grid and optimize: replace whole space by N points $\{x_1, \ldots, x_N\}$

$$\rho \approx \sum_{i=1}^{N} p_i \delta_{x_i}$$

Cons: Curse of dimensionality

Literature Review on Infinite-Dimensional Optimization

$$\min_{\rho \in \mathscr{P}(\mathbb{R}^d)} \quad \mathscr{F}(\rho)$$

1. Grid and optimize
2. Duality [Shapiro A, etc...]

Cons: Specialize to problem structures

Literature Review on Infinite-Dimensional Optimization

$$\min_{\rho \in \mathscr{P}(\mathbb{R}^d)} \quad \mathscr{F}(\rho)$$

1. Grid and optimize
2. Duality
3. Frank-wolfe algorithm **[Jaggi M, 2013]**:
   Iteratively,

Cons: Subproblems are generally difficult to solve

$$\nu = \operatorname*{argmin}_{\mu \in \mathscr{P}} \mathscr{F}'_{\mu}(\mu_k), \mu_{k+1} = (1-\beta)\mu_k + \beta\nu$$

Literature Review on Infinite-Dimensional Optimization

$$\min_{\rho \in \mathscr{P}(\mathbb{R}^d)} \quad \mathscr{F}(\rho)$$

1. Grid and optimize
2. Duality
3. Frank-wolfe algorithm
4. Particle Gradient Descent **[Chizat L, Bach F, 2018]**

Cons: Sharp convergence generally applicable to entropic regularized objective

Initialize $\mu = \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}$, update particles $\{x_i\}_i$ using gradient descent

Sinkhorn Discrepancy

$$\mathcal{W}_\epsilon(\mathbb{P},\mathbb{Q}) = \inf_{\gamma\in\Gamma(\mathbb{P},\mathbb{Q})} \left\{ \mathbb{E}_{(x,y)\sim\gamma}[\|x-y\|^2] + \epsilon\mathbb{E}_{(x,y)\sim\gamma}\left[\log\left(\frac{\mathrm{d}\gamma(x,y)}{\mathrm{d}\gamma(x)\mathrm{d}y}\right)\right]\right\}$$

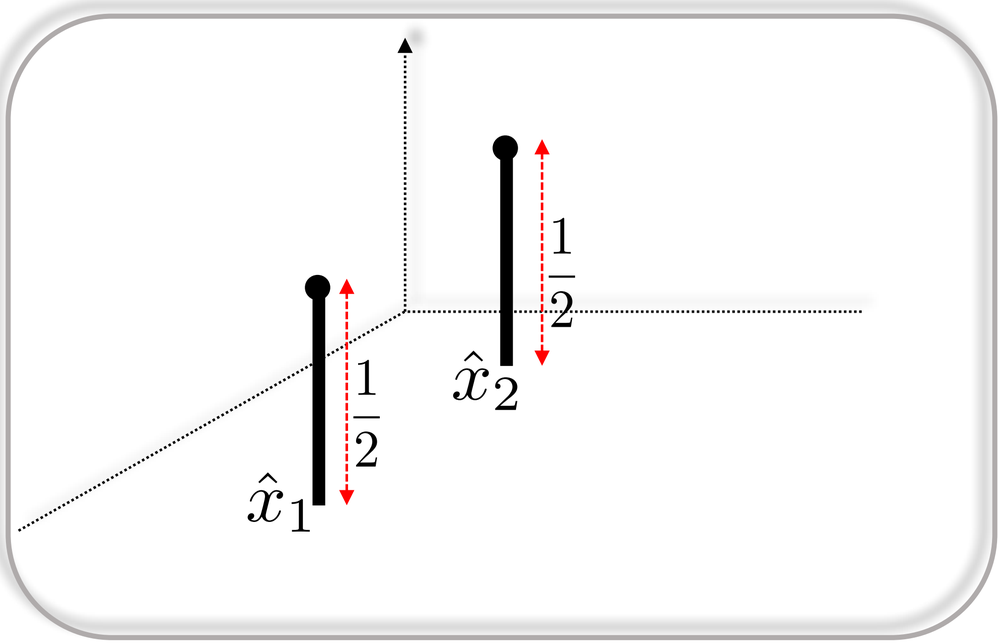
Historical Review:

- Originally proposed by [Wilson' 62]
- Convergence of algorithm for the first time by [Sinkhorn' 64]
- Operation complexity analysis and practical application by [Cuturi' 13, ...]

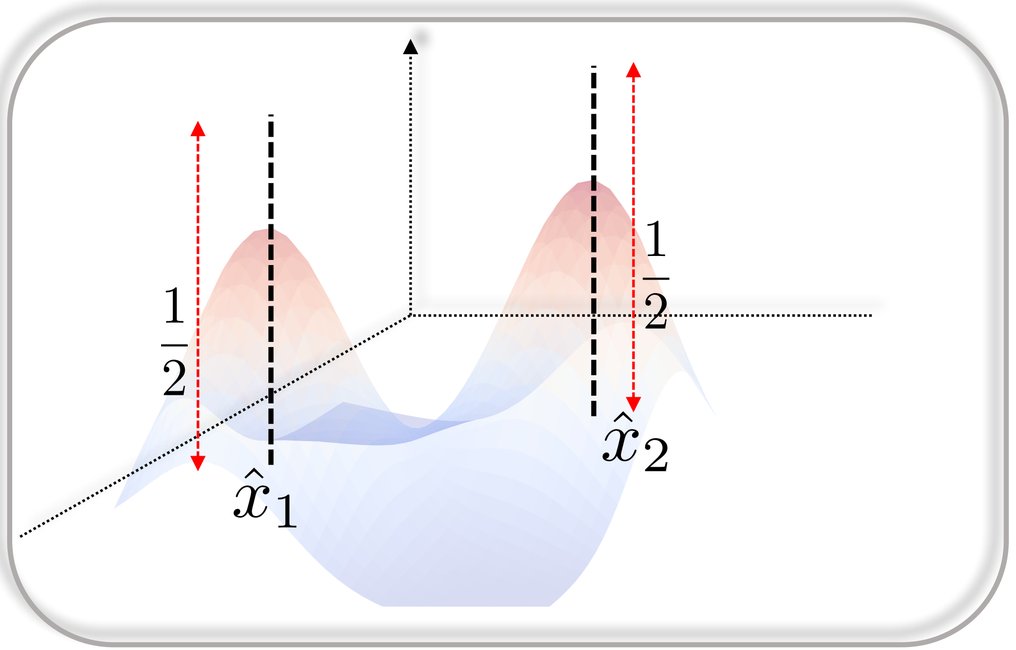
Main Framework

Sinkhorn DRO: $\min_{\theta} \left\{ \sup_{\mathbb{P}:\ \mathcal{W}_\epsilon(\mathbb{P}_n, \mathbb{P}) \le \rho} \mathbb{E}_{z\sim\mathbb{P}}[\ell(z;\theta)] \right\}$

$$\mathcal{W}_\epsilon(\mathbb{P},\mathbb{Q}) = \inf_{\gamma\in\Gamma(\mathbb{P},\mathbb{Q})} \left\{ \mathbb{E}_{(x,y)\sim\gamma}[\|x-y\|^2] + \epsilon \mathbb{E}_{(x,y)\sim\gamma}\left[\log\left(\frac{\mathrm{d}\gamma(x,y)}{\mathrm{d}\gamma(x)\mathrm{d}y}\right)\right] \right\}$$



Empirical Distribution



Worst-case distribution by Sinkhorn DRO

Strong Dual Reformulation

Under mild conditions, $V_{\text{Primal}}=V_{\text{dual}}$:

$$V_{\text{Primal}} = \sup_{\mathbb{P}} \left\{ \mathbb{E}_{z\sim\mathbb{P}}[\ell(z;\theta)] : \ \mathcal{W}_\epsilon(\mathbb{P}_n, \mathbb{P}) \le \rho \right\}$$

$$V_{\text{Dual}} = \inf_{\lambda\ge 0} \left\{ \lambda\bar{\rho} + \mathbb{E}_{x\sim\mathbb{P}_n}\left[\lambda\epsilon \log \mathbb{E}_{z\sim\mathbf{N}(x,\epsilon\mathbf{I})}[e^{\ell(z;\theta)/(\lambda\epsilon)}]\right] \right\}$$

- $\bar{\rho} = \rho + \epsilon\mathbb{E}_{x\sim\mathbb{P}_n}[\log(\int e^{-\|x-z\|^2/\epsilon}\mathrm{d}z)]$
- V_{dual} : **One-dimensional convex** minimization, **conditional stochastic optimization**

Monte Carlo Sampling

$$\min_{\theta,\lambda\geq 0}\left\{\lambda\bar{\rho}+\mathbb{E}_{x\sim\mathbb{P}_n}\left[\lambda\epsilon\log\mathbb{E}_{z\sim\mathbf{N}(x,\epsilon\mathbf{I})}\left[e^{\ell(z;\theta)/(\lambda\epsilon)}\right]\right]\right\}$$

- Jie Wang, Rui Gao, Yao Xie (2025) Sinkhorn Distributionally Robust Optimization. *Operations Research*

Monte Carlo Sampling

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"As long as you can sample from $\mathbb{P}_n$ and $\mathbf{N}(x, \epsilon\mathbf{I})$, the problem is solved".

- A. Shapiro

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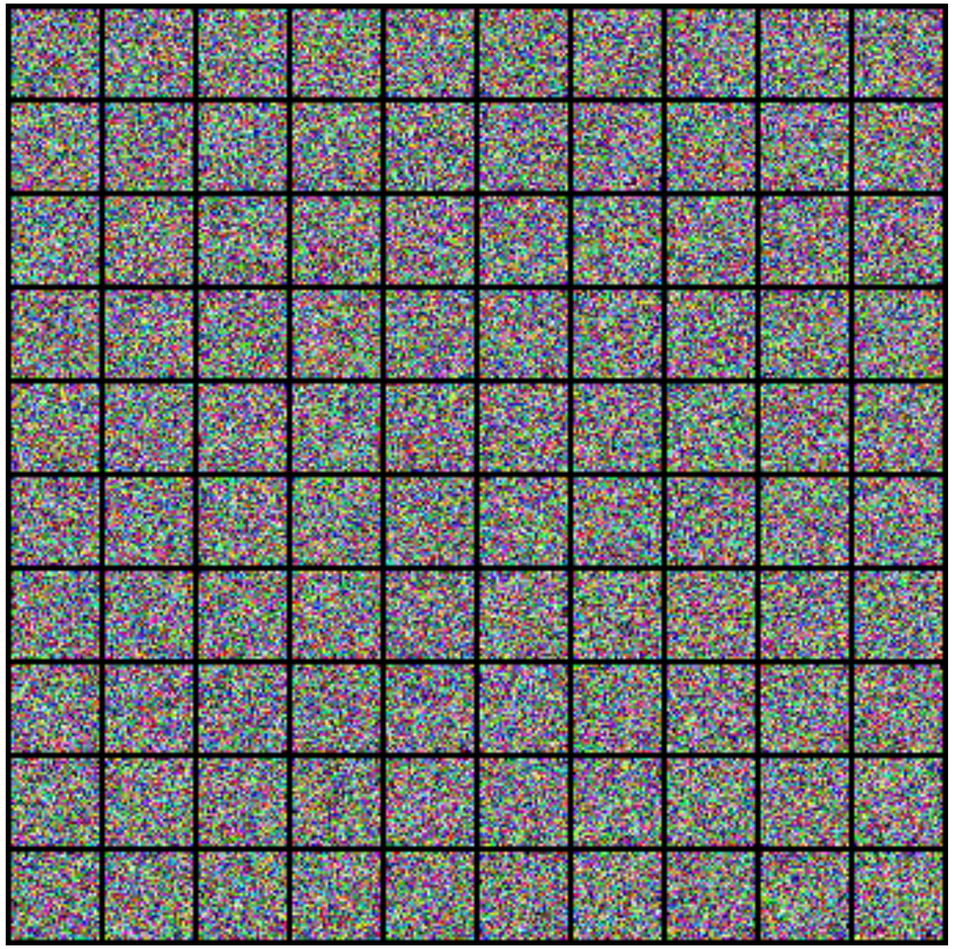
Diffusion Model



- Given training samples $\{x^{(1)}, \ldots, x^{(n)}\}$ i.i.d. from $\mathbb{P}_{\text{true}}$
- **Goal of Generative AI**: Generate a sample $\hat{x}$ with distribution close to $\mathbb{P}_{\text{true}}$
  - Step 1: Learn score function $s(x) \approx \log \mathbb{P}_{\text{true}}(x)$;
  - Step 2: Sampling from (unnormalized density) $\exp(s(x))$ using Langevin dynamics.

Song, Y., Sohl-Dickstein, J., Kingma, D. P., Kumar, A., Ermon, S., & Poole, B. Score-Based Generative Modeling through Stochastic Differential Equations. In *International Conference on Learning Representations*.

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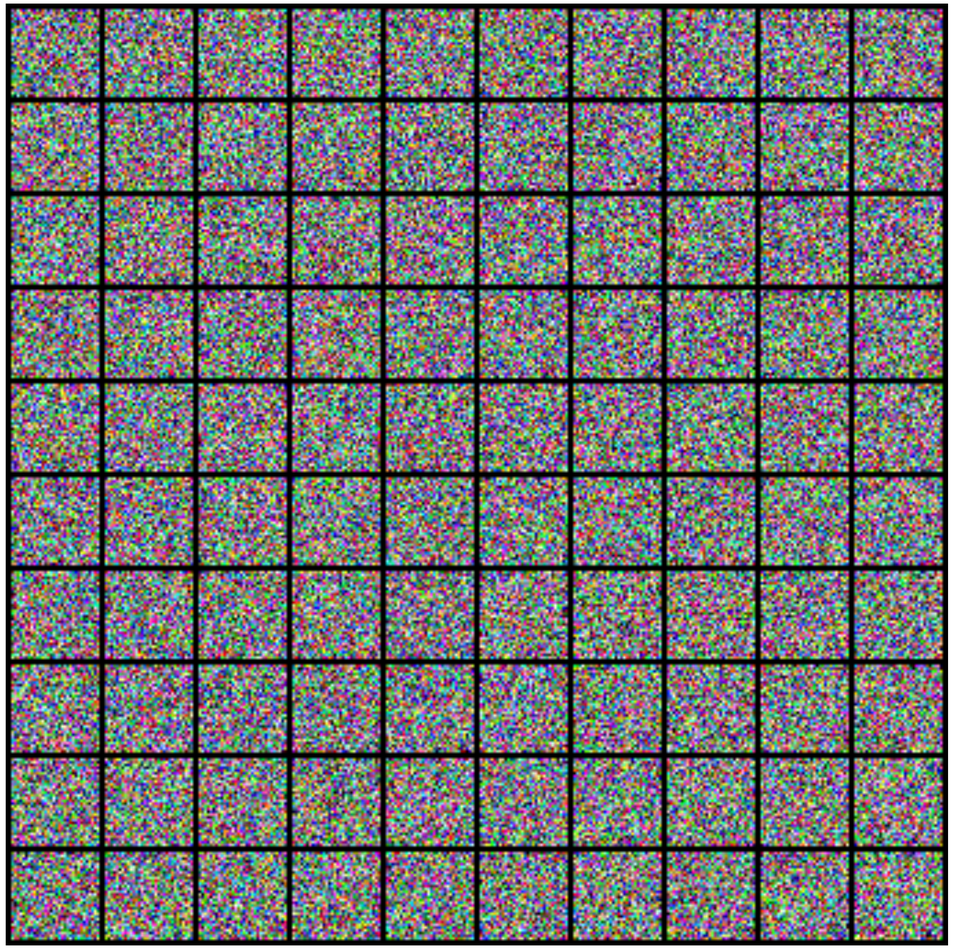

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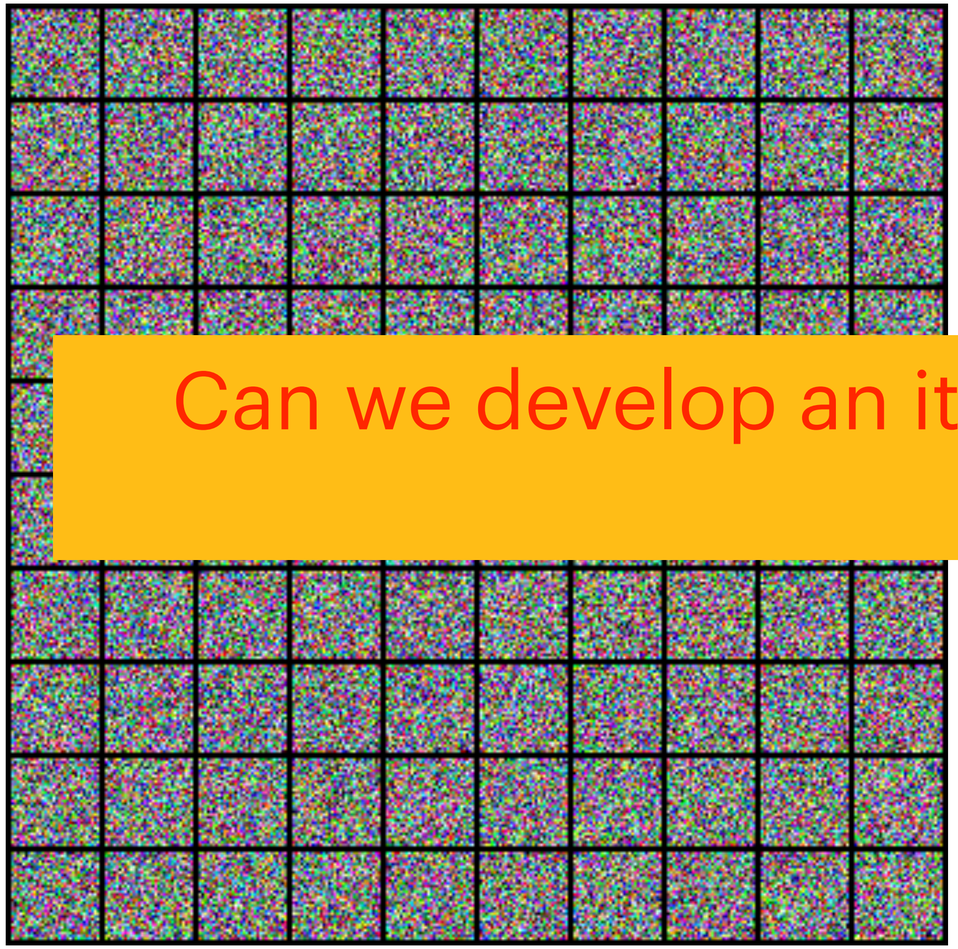

- Given training samples $\{x^{(1)}, \ldots, x^{(n)}\}$ i.i.d. from $\mathbb{P}_{\text{true}}$
- **Goal of Generative AI**: Generate a sample

Can we develop an iterative sampling approach to solving Sinkhorn DRO?

$s(x) \approx \log \mathbb{P}_{\text{true}}(x)$;

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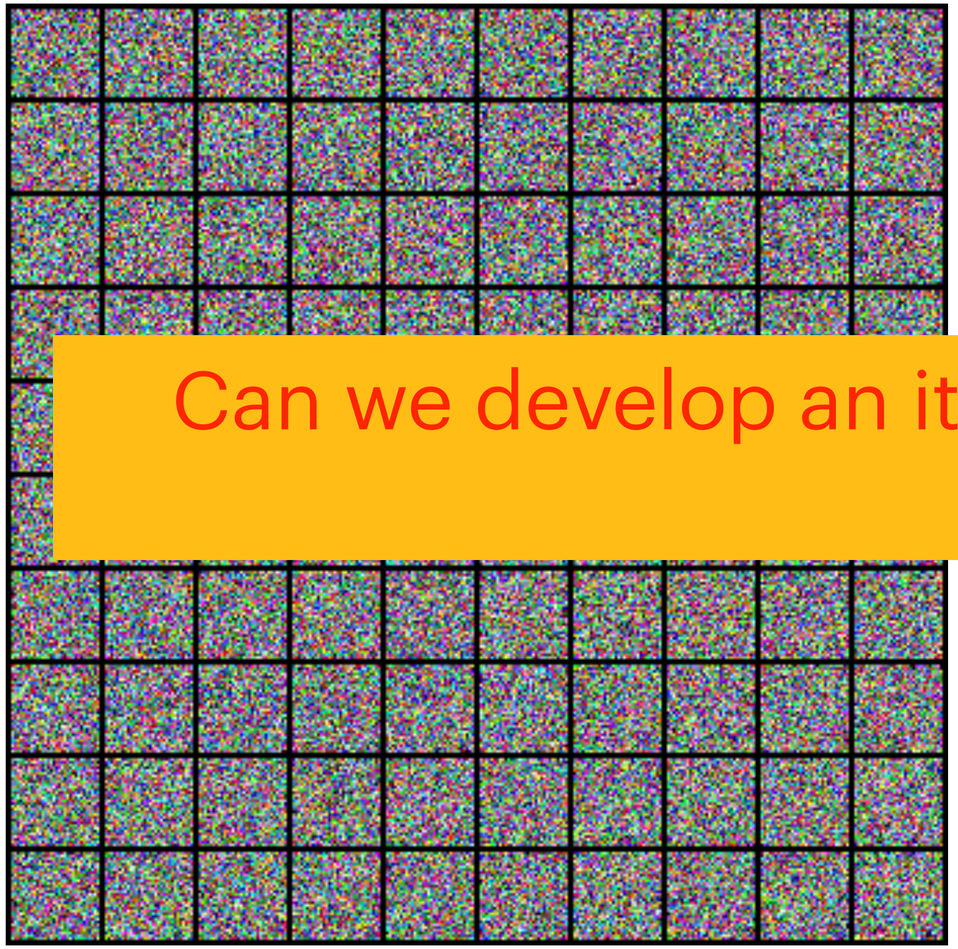

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Diffusion for Sinkhorn DRO

$$\min_{\theta} \ \mathbb{E}_{z\sim\mathbb{P}^*_\theta}[\ell(\theta; z)]$$

where $\mathbb{P}^*_\theta = \frac{1}{n}\sum_{i\in[n]} \mathbb{P}^*_{i,\theta}$

and $$\boxed{\frac{\mathrm{d}\mathbb{P}^*_{i,\theta}}{\mathrm{d}z}(z) \propto \exp\left(\frac{\ell(z;\theta)}{\lambda\epsilon} - \frac{\|x^{(i)} - z\|_2^2}{2\epsilon}\right)}$$

Efficient sampling from $\mathbb{P}^*_{i,\theta}$ requires **log-Sobolev inequality (LSI)**

If converged?

False

Sample $i \in [n]$ and next sample $z \sim \mathbb{P}^*_{i,\theta}$

Generate gradient estimator $\nabla\ell(\theta, z)$ and update θ

Sampling via Langevin Dynamics

$$\frac{\mathrm{d}\mathbb{P}^*_{i,\theta}}{\mathrm{d}z}(z) \propto \exp\left(\frac{\ell(z;\theta)}{\lambda\epsilon} - \frac{\|x^{(i)} - z\|_2^2}{2\epsilon}\right)$$

$$\mathbb{P}^*_{i,\theta} = \mathrm{argmax}_{\mathbb{P}} \left\{ \mathbb{E}_{z\sim\mathbb{P}}[\ell(z;\theta)] - \frac{\lambda}{2}\mathbb{E}_{z\sim\mathbb{P}}[\|z - x^{(i)}\|_2^2] - \lambda\epsilon\mathscr{H}(\mathbb{P}) \right\}$$

$$z_{k+1} = z_k + \eta \cdot \left(\nabla_z \ell(z;\theta) - \lambda(z - x^{(i)})\right) + \sqrt{2\eta\lambda\epsilon} \cdot \mathbf{N}(0, I_d)$$

Demo

$$\min_{\theta} \left\{ \sup_{\mathbb{P}:\ \mathcal{W}_\epsilon(\mathbb{P}_n, \mathbb{P}) \leq \rho} \mathbb{E}_{z\sim\mathbb{P}}[\ell(z;\theta)] \right\}$$

- $\ell(z;\theta)$ is a convolutional neural net with logistic loss
- Classification task with 5 samples from MNIST digit 3 and 5 samples from digit 8

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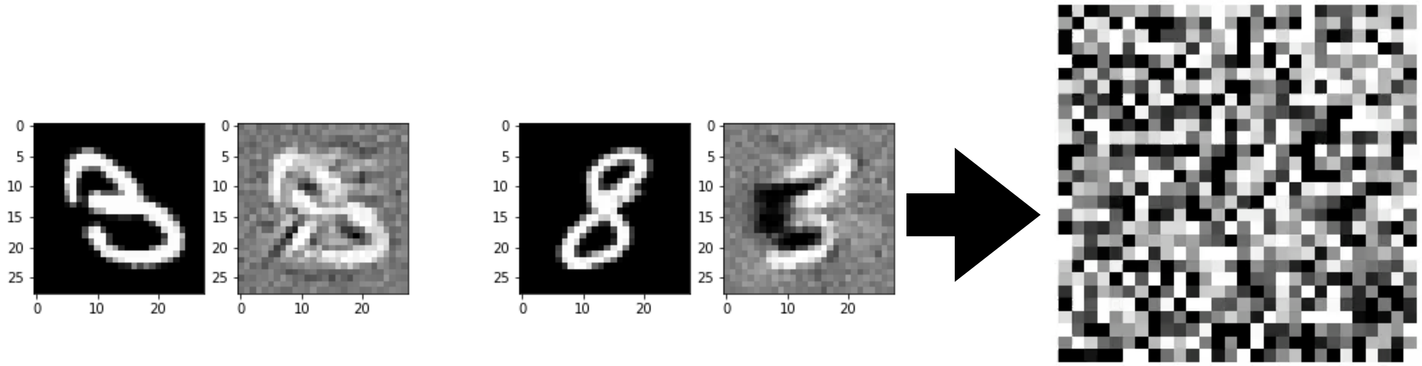

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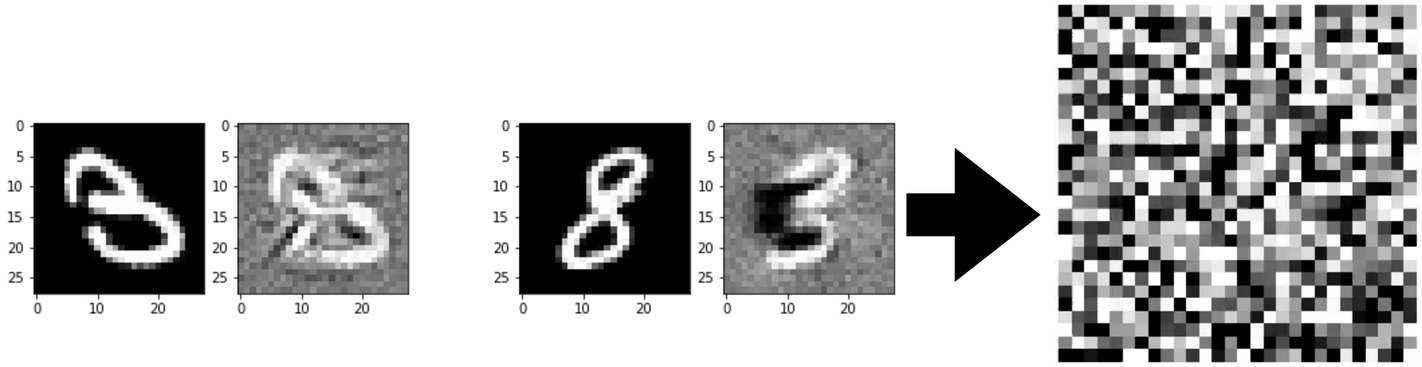

1. Sinkhorn DRO can be viewed as a "task-aware" generative AI (GenAI)
2. Conventional GenAI: target distribution is given as a *priori*

Bilevel Reformulation for Sinkhorn DRO

$$\min_{\theta} \; F(\theta) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\mu_{i,\theta}^*}[\ell(z;\theta)]$$

$$\mu_{i,\theta}^* = \operatorname*{argmin}_{\mu \in \mathscr{P}} \mathscr{D}_{\mathrm{KL}}\big(\mu \| u_{i,\theta}(\,\cdot\,)\big), \quad i \in [n]$$

$$u_{i,\theta}(z) \propto \exp\left(\frac{\ell(z;\theta)}{\lambda\epsilon} - \frac{1}{2\epsilon}\|z - x^{(i)}\|_2^2\right)$$

Double Loop Algorithm:
Iteratively,

1. Fix upper-level decision
2. Run inner-loop to find near-optimal lower-level solution
3. Update upper-level solution

For large n, randomly select a batch of lower-level problems

Bilevel Reformulation for Sinkhorn DRO

$$\min_{\theta} \; F(\theta) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\mu^*_{i,\theta}}[\ell(z;\theta)]$$

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Single Loop Algorithm:
Iteratively,

1. Fix upper-level decision
2. One-step update of lower-level solution
3. One-step update of upper-level solution

Randomly update a batch of lower-level problem solutions, leave others unchanged.

Bilevel Reformulation for Sinkhorn DRO

$$\min_{\theta} \; F(\theta) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_{\mu^*_{i,\theta}}[\ell(z;\theta)]$$

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Single Loop Algorithm:
Iteratively,

1. Fix upper-level decision
2. One-step update of lower-level solution
3. One-step update of upper-level solution

- Generate gradient estimator for upper-level solution,
- Construct a moving average estimator,
- Do the update.

Single-Loop Algorithm for Sinkhorn DRO

Algorithm 3 Mean-Field Single-Loop Iterative Sampling Algorithm

Require: Stepsize parameters η, τ, initial guess $\mu_0^{(i)}, i \in [n]$, moving average estimator r_0, moving average parameter β_0, number of iterations T.

for $k = 0, 1, 2, \ldots, T-1$ **do**
  Randomly sample indices $I_k \subseteq [n]$
  for $i \in [n]$ **do**
    Update $\mu_{k+1}^{(i)}$ according to (10)
  end for
  Update gradient estimator v_{k+1} according to (11)
  Update $r_{k+1} = (1-\beta_0) r_k + \beta_0 v_{k+1}$
  Update $\theta_{k+1} = \theta_k - \tau \eta r_{k+1}$.
end for
Output $\widehat{\theta}$ uniformly selected from $\{\theta_1, \ldots, \theta_T\}$.

Convergence Analysis

Under LSI assumption on worst-case distribution, it holds that:

Double-loop algorithm finds ϱ-stationary solution with complexity $\mathcal{O}(\varrho^{-6})$.

- Solving Sinkhorn DRO from the dual requires boundness of loss function $\ell(z;\theta)$
- Existing algorithm has complexity $\mathcal{O}(\varrho^{-4})$ **[Hu et. al 2023]** by Multi-level Monte Carlo Technique.

Convergence Analysis

Under LSI assumption on worst-case distribution, it holds that:

Single-loop algorithm finds ϱ-stationary solution with complexity $\mathcal{O}(\varrho^{-6})$.

Proof Outline

Lemma 4.2 (Descent Lemma). *Assume Assumption 3.6(II) holds and the stepsize parameters satisfy* $\eta\tau \leq \frac{1}{2L_{f,2}}$. *Consider the update in Step 8 of Algorithm 3, it holds that*

$$F(\theta_{k+1}) \leq F(\theta_k) + \frac{\tau\eta}{2}\|\nabla F(\theta_k) - r_{k+1}\|_2^2 - \frac{\tau\eta}{2}\|\nabla F(\theta_k)\|_2^2 - \frac{\tau\eta}{4}\|r_{k+1}\|_2^2.$$

Critical Step: Bound the difference between **true hypergradient** $\nabla F(\theta_k)$ and our **gradient estimator** r_{k+1} used in k-th iteration

Proof Outline

Lemma 4.3 (Gradient Difference Lemma). *Assume Assumption 3.6(II) holds, and the parameter* $\beta_0 \in (0, 1]$, *then it holds that*

$$\begin{aligned}\mathbb{E}\left[\|\nabla F(\theta_k) - r_{k+1}\|_2^2 \middle| \mathcal{G}_{k-1}\right] \leq (1-\beta_0)\|\nabla F(\theta_{k-1}) - r_k\|_2^2 + \frac{4L_{f,2}^2\tau^2\eta^2}{\beta_0}\|r_k\|_2^2 \\ + 4\beta_0\left\|\nabla F(\theta_k) - \nabla F(\theta_k; \mu_k^{(1:n)})\right\|_2^2 + \beta_0^2\mathbb{E}\left[\left\|\nabla F(\theta_k; \mu_k^{(1:n)}) - v_{k+1}\right\|_2^2 \middle| \mathcal{G}_{k-1}\right].\end{aligned} \tag{13}$$

On the right-hand-side of (13), it can be shown that the last component can be bounded in terms of the variance of v_{k+1}, and the third component can be bounded as

$$\left\|\nabla F(\theta_k) - \nabla F(\theta_k; \mu_k^{(1:n)})\right\|_2^2 \leq \frac{L_{f,1}^2}{n}\sum_{i\in[n]}\mathcal{D}_{\mathrm{KL}}(\mu_k^{(i)}, \mu_*^{i,\theta_k}).$$

Major Difficulty: Bound difference between true lower-level solution μ_*^{i,θ_k} and estimated lower-level solution $\mu_k^{(i)}$

Proof Outline

Lemma 4.4 (KL-Divergence Bound). *Assume Assumptions 3.2 and 3.6 hold, then it holds that*

$$\sum_{k=0}^{T} \mathbb{E}\left[\mathcal{D}_{\mathrm{KL}}(\mu_k^{(i)} \| \mu_*^{i,\theta_k})\right]$$

$$\leq \frac{4n}{\alpha\tau|I_k|}\mathcal{D}_{\mathrm{KL}}(\mu_0^{(i)} \| \mu_*^{i,\theta_0}) + \frac{12\eta L_{f,1}^2 Tn}{\lambda\epsilon\alpha|I_k|} + \frac{32\tau\epsilon d L_{G,2}^2 T}{\alpha} + \frac{20\eta n}{\lambda\epsilon\alpha|I_k|}\sum_{k=0}^{T-1}\mathbb{E}\left[\|r_{k+1}\|_2^2\right].$$

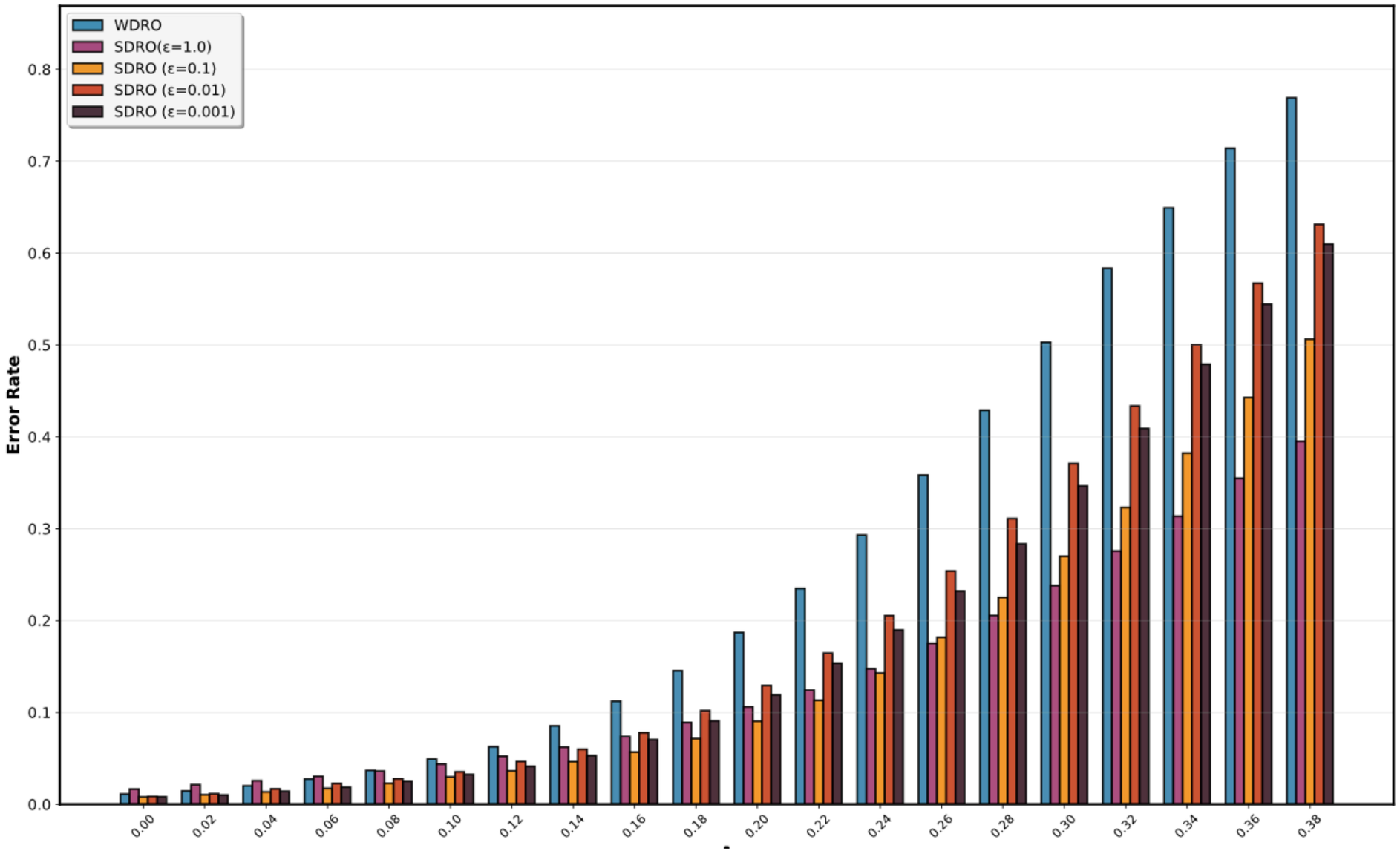
- Many tricks in finite-dimensional bilevel program are **not applicable**, e.g., triangular inequality
- Use KL-divergence as a metric. Analyze the trajectory

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{D}_{\mathrm{KL}}(\rho_t \| \mu_*^{i,\vartheta_t})$$

$$\vartheta_t = \theta_k - t\eta r_{k+1}$$

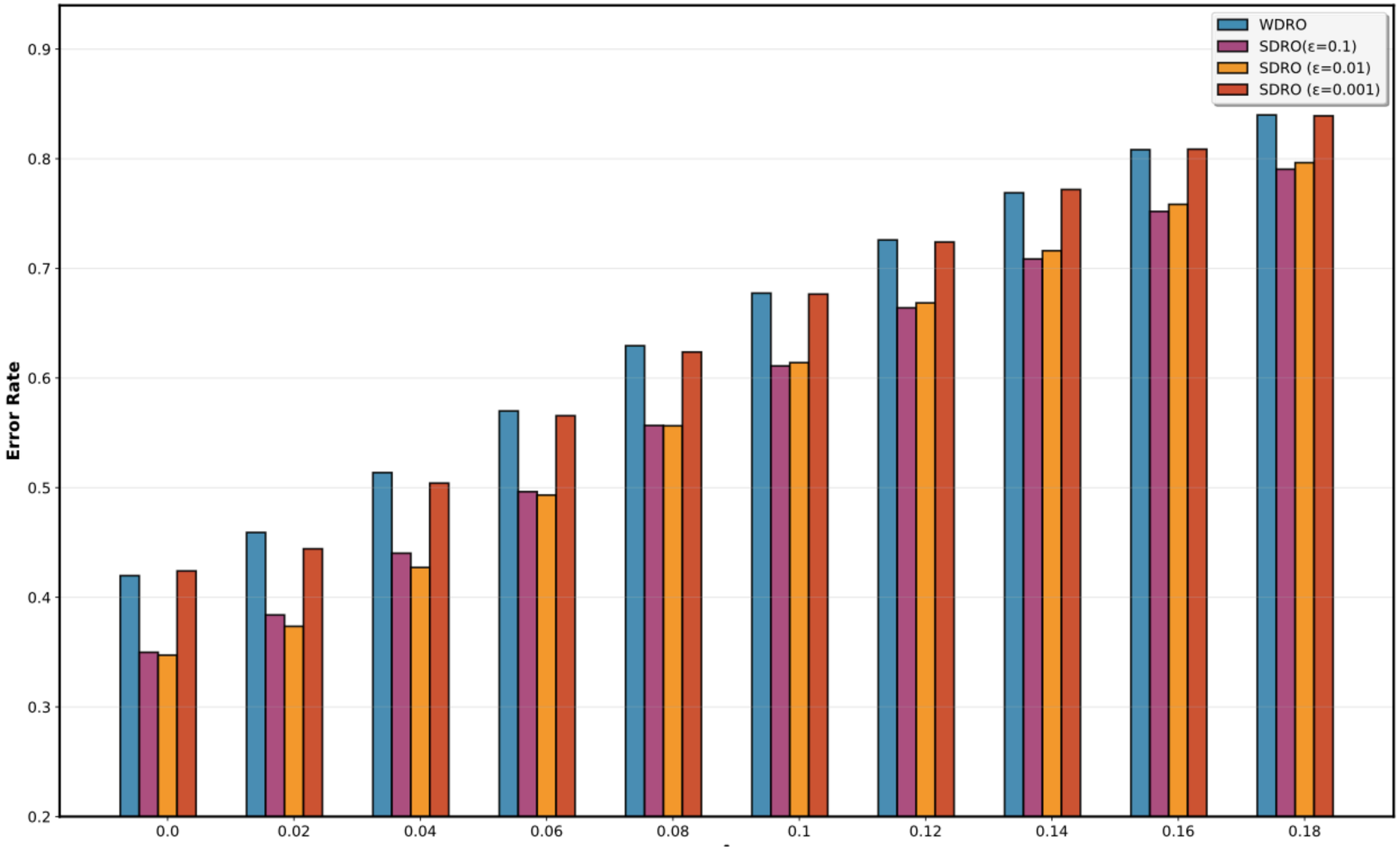
$$\mathrm{d}z_t = -\left(-\frac{\nabla f_{\theta_k}(z_t)}{\lambda} + (z_t - x^{(i)})\right)\mathrm{d}t + \sqrt{2\epsilon}\mathrm{d}\mathbf{W}_t, \quad \mathrm{Law}(z_t) = \rho_t, \rho_0 = \mu_k^{(i)}, \rho_\tau = \mu_{k+1}^{(i)}$$

Numerical Study



- MNIST Dataset
- *x*-axis: level of perturbation
- *y*-axis: error rate on testing dataset

Numerical Study



- CIFAR-10 Dataset
- *x*-axis: level of perturbation
- *y*-axis: error rate on testing dataset

Summary

- Solving Sinkhorn DRO from the **primal perspective**
- Reformulate Sinkhorn DRO as **infinite-dimensional bilevel program** with **multiple lower-level problems**.
- Double-loop algorithm is a "**noisy**" counterpart of the Wasserstein DRO algorithm by **[Sinha et. al 2018]**
- Single-loop algorithm requires **ODE analysis** in addition to finite-dimensional optimization tricks.