## Asymptotic Normality and Confidence Regions in Wasserstein Distributionally Robust Optimization

#### Nian Si Joint work with Jose Blanchet and Karthyek Murthy

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1 [Introduction to DRO and optimal transport](#page-2-0)



2 [Asymptotic behaviors and confidence regions of DRO estimators](#page-14-0)

### **Motivation**

<span id="page-2-0"></span>

Stochastic optimization problem:

 $\inf_{\beta \in \mathbb{R}^d} \mathbb{E}_{P_*}[\ell(X;\beta)],$ 

 $P_*$ : Ground truth distribution,  $\odot$  usually unknown in practice.

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<span id="page-3-0"></span> $\inf_{\beta \in \mathbb{R}^d} \mathbb{E}_{P_n}[\ell(X; \beta)],$ 

 $P_n$ : Empirical distribution.

 $\circled{c}$  : Overfitting  $\Rightarrow$  poor out-of-sample performance.

 $\circled{c}$  : Non-robustness  $\Rightarrow$  adversarial examples [Goodfellow et al., 2014].

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#### Robust data-driven framework.

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## DRO formulation

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#### Distributionally Robust Optimization (DRO):

$$
\inf_{\beta \in \mathbb{R}^d} \sup_{\substack{P \in \mathcal{U} \\ \text{worst case expectation}}} \mathbb{E}_P[\ell(X; \beta)],
$$

 $U:$  distributional uncertainty set.

## DRO formulation

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Construction of distributional uncertainty set  $\mathcal{U}$ :

$$
\mathcal{U}=\mathcal{U}_{\delta}(P_n)=\{P\in\mathcal{P}(S):D(P,P_n)\leq\delta\}
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Choices of  $D(\cdot, \cdot)$ : f – divergence, optimal transport cost

## DRO formulation

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### Literatures on DRO

<span id="page-8-0"></span>

- **f-divergence:** [Bagnell, 2005; Ben-Tal et al., 2013; Bertsimas, Gupta  $\&$ Kallus, 2013; Hu & Hong 2013; Lam, 2013; 2016; Wang, Glynn & Ye, 2014; Bayrakskan & Love, 2015; Duchi, Glynn & Namkoong, 2016; Duchi & Namkoong, 2016; 2017]
- **Optimal transport:** [Esfahani & Kuhn, 2018; Blanchet & Murthy, 2019; Gao & Kleywegt, 2016; Blanchet, Kang & Murthy, 2016; Gao, Chen & Kleywegt, 2017; Sinha, Namkoong & Duchi, 2017; Nguyen, Kuhn & Esfahani, 2018; Nguyen et al., 2018; Blanchet et al., 2019]

### Optimal transport

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- Let  $P \in \mathcal{P}(S)$  and  $Q \in \mathcal{P}(S)$  be two probability distributions defined on a space  $S$ ;  $c : S \times S \rightarrow [0, \infty]$  is a cost function.
- Optimal transport cost:

$$
D_c(P,Q) = \inf_{\pi} \{ \mathbb{E}_{\pi}[c(U,V)] \mid \pi \in \mathcal{P}(S \times S), \pi_U = P, \pi_V = Q \}
$$

### Optimal transport

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- Advantages:
	- $\bullet$  P and Q are not required to have the same support;
	- Continuous distributions are included;
	- General enough to cover popular distances used in practice,  $c(u,v)=\|u-v\|^{\rho}\Longrightarrow D_{c}^{1/\rho}:\rho\text{-Wasserstein distance};$  $c(u, v) = \mathbf{1}{u \neq v} \Longrightarrow D_c$ : total variation distance.

#### DRO estimators

#### **• Square-root LASSO** [Belloni, Chernozhukov and Wang 2011]:

<span id="page-11-0"></span>
$$
\ell((x, y); \beta) = ||y - \beta^{T} x||_{2}^{2}
$$

$$
P_{n} = \frac{1}{n} \sum_{i=1}^{n} \delta_{(X_{i}, Y_{i})}(dx, dy)
$$

$$
c((x, y), (x', y')) = ||x - x'||_{q}^{2} + \infty \cdot \mathbf{1}{y \neq y'}
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DRO is equivalent to the square-root LASSO [Blanchet, Kang and Murthy, 2016],  $(1/p+1/q=1)$  $\Omega$ 

<span id="page-12-0"></span>
$$
\sup_{P:D_c(P,P_n)\leq \delta} \mathbb{E}_P\left[\ell((X,Y);\beta)\right] = \left(\sqrt{\mathbb{E}_{P_n}[\ell((X,Y);\beta)]} + \sqrt{\delta} \|\beta\|_p\right)^2.
$$

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$$

• Regularized logistic regression, SVMs...



<span id="page-14-0"></span>





2 [Asymptotic behaviors and confidence regions of DRO estimators](#page-14-0)

### • The asymptotic behaviors of DRO estimators? Suppose  $X_1, X_2, \ldots, X_n \stackrel{i.i.d.}{\sim} P_*$ ,

<span id="page-15-0"></span>
$$
\beta_n^{ERM} \in \arg\min_{\beta} \mathbb{E}_{P_n} [\ell(X;\beta)],
$$
  

$$
\beta_n^{DRO}(\delta) \in \arg\min_{\beta} \sup_{P \in \mathcal{U}_{\delta}(P_n)} \mathbb{E}_{P_n} [\ell(X;\beta)],
$$
  

$$
\beta_* = \arg\min_{\beta} \mathbb{E}_{P_*} [\ell(X;\beta)].
$$

We want to study the joint limit of  $(n^{1/2}(\beta_n^{ERM}-\beta_*),n^?(\beta_n^{DRO}(\delta_n)-\beta_*))$  with the correct scaling rate.

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We want to study the joint limit of  $(n^{1/2}(\beta_n^{ERM}-\beta_*),n^?(\beta_n^{DRO}(\delta_n)-\beta_*))$  with the correct scaling rate.

#### • The suitable confidence regions in DRO problems? We want to find a confidence region  $\Lambda_n$  that

<span id="page-16-0"></span>
$$
\beta_n^{ERM} \in \Lambda_n, \ \beta_n^{DRO}(\delta_n) \in \Lambda_n \text{ and } \lim_{n \to \infty} \mathbf{P}(\beta_* \in \Lambda_n) = 1 - \alpha.
$$

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• Define "Compatible" set as

$$
\Lambda_{\delta_n}(P_n):=\left\{\beta\in\mathbb{R}^d: \beta\in\arg\min_{\beta}\mathbb{E}_{P}\left[\ell(X;\beta)\right] \textrm{ for a } P\in\mathcal{U}_{\delta_n}(P_n)\right\}.
$$

- $\Lambda_{\delta_n}(P_n)$  denotes the set of choices of  $\beta\in\mathbb{R}^d$  that are "compatible" with the distributional uncertainty region, in the sense that for every  $\beta\in \Lambda_{\delta_n}(P_n),$  there exists a probability distribution  $P\in \mathcal{U}_{\delta_n}(P_n)$  for which  $\beta$  is optimal.
- $\Lambda_{\delta_n}(P_n)$  naturally serves as a good candidate of confidence regions.

### Preliminaries

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- We consider the cost function with the form  $c(u,w) = ||u w||_q^2$ q .
- Let  $h(x, \beta) := D_{\beta} \ell(x, \beta)$  be the gradient of the loss function and  $C := \mathbb{E} \left[ D_{\beta} h(X, \beta_{*}) \right] \succ \mathbf{0}.$
- **o** Define

$$
\varphi(\xi) := \frac{1}{4} \mathbb{E}_{P_*}\left( \left\| \left(D_{\mathsf{x}} h(X,\beta_*)\right)^{\mathsf{T}} \xi \right\|_{\rho}^2 \right),\,
$$

where  $1/p + 1/q = 1$  and its convex conjugate:

$$
\varphi^*(\zeta):=\sup_{\xi\in\mathbb{R}^d}\left\{\xi^{\mathcal{T}}\zeta-\varphi(\xi)\right\}.
$$

**o** Define

<span id="page-18-0"></span>
$$
\mathcal{S}(\beta) := \sqrt{\mathbb{E}_{P_*} ||D_{\mathsf{x}} \ell(X;\beta)||_p^2}.
$$

## Main asymptotic theorem

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#### Theorem (Main theorem)

Suppose  $\ell$  (x, ·) is convex and  $\ell$  (·) satisfies mild regularity conditions. Let  $\delta_n = n^{-\gamma} \eta$  for  $\gamma, \eta \in (0, \infty)$ , and  $H \sim \mathcal{N}(\mathbf{0}, \text{Cov}[h(X, \beta_*)])$ . Then,

$$
\left(n^{1/2}(\beta_n^{ERM}-\beta_*)\, , n^{\bar{\gamma}/2}(\beta_n^{DRO}(\delta_n)-\beta_*), n^{1/2}\left(\Lambda_{\delta_n}(P_n)-\beta_*\right)\right)
$$
  
\n
$$
\Rightarrow \left(C^{-1}H, C^{-1}f_{\eta,\gamma}(H), \Lambda_{\eta,\gamma}+C^{-1}H\right),
$$

where  $\bar{\gamma} := \min \{ \gamma, 1 \}$  and  $f_{n,\gamma}(x), \Lambda_{n,\gamma}$  will be defined later according to  $\gamma$ .

## Main asymptotic theorem : Remarks

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This theorem works for every scaling rate  $\delta_{\bm n} = \eta / \bm n^\gamma, \gamma > 0$ . However, only  $\delta_n = \eta/n$  gives the non-trivial limits.

## Main asymptotic theorem : Remarks

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$$
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 $\gamma>1$ : Lack of robustness.  $\beta^{DRO}_{n}$  and  $\beta^{ERM}_{n}$  are asymptotically indistinguishable,

$$
n^{1/2}\left((\beta_n^{ERM}-\beta_*) ,(\beta_n^{DRO}(\delta_n)-\beta_*),(\Lambda_{\delta_n}(P_n)-\beta_*)\right) \Rightarrow \left(C^{-1}H,C^{-1}H,\{C^{-1}H\}\right).
$$

## Main asymptotic theorem : Remarks

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$$

 $\bullet \ \gamma < 1$ : Excessive robustness. Slow convergence rate and an asymptotically bias,

$$
\left(n^{\gamma/2}(\beta_n^{DRO}(\delta_n)-\beta_*),n^{1/2}(\Lambda_{\delta_n}(P_n)-\beta_*)\right)\Rightarrow\left(-\sqrt{\eta}C^{-1}D_{\beta}S(\beta_*),\mathbb{R}^d\right).
$$

### Main asymptotic theorem :  $\gamma = 1$



•  $\gamma = 1$ : non-trivial limits.

$$
n^{1/2} \left( (\beta_n^{ERM} - \beta_*) , (\beta_n^{DRO}(\delta_n) - \beta_*), (\Lambda_{\delta_n}(P_n) - \beta_*) \right)
$$
  
\n
$$
\Rightarrow (C^{-1}H, C^{-1}H - \sqrt{\eta}C^{-1}D_{\beta}S(\beta_*), \{u : \varphi^*(Cu) \leq \eta\} + C^{-1}H).
$$

• Here,  $\Lambda_{n,1}$  is defined by

<span id="page-23-0"></span>
$$
\Lambda_{\eta,1}=\{u:\varphi^*(Cu)\leq\eta\}\,.
$$

### Confidence regions:  $\delta_n = n/n$

<span id="page-24-0"></span>

DRO solution is inside the "compatible" set  $(\beta_n^{DRO}(\delta_n) \in \Lambda_{\delta_n}(P_n))$ , because of the proposition below.

#### Proposition (Blanchet et.al., 2016)

If  $\ell$   $(x, \cdot)$  is convex, we have for any  $\delta > 0$ ,

 $\inf_{\beta}$  sup<br> $\frac{\beta}{\beta}$  P:D(P<sub>ar</sub>)  $P:D(P_n,P) \leq \delta$  $\mathbb{E}_{P}\left[\ell(X;\beta)\right] = \quad \textsf{sup}$  $P:D(P_n,P) \leq \delta$  $\inf_{\beta} \mathbb{E}_{P} [\ell(X; \beta)].$ 

## Confidence regions:  $\delta_n = n/n$

<span id="page-25-0"></span>
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\underset{\text{University}}{Stanford}
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\inf_{\beta} \sup_{P:D(P_n,P) \leq \delta} \mathbb{E}_{P} \left[ \ell(X;\beta) \right] = \sup_{P:D(P_n,P) \leq \delta} \inf_{\beta} \mathbb{E}_{P} \left[ \ell(X;\beta) \right].
$$

 $\Lambda_{\delta_n}(P_n)$  has exact asymptotic coverage.

$$
\lim_{n \to \infty} \mathbf{P}(\beta_* \in \Lambda_{\delta_n}(P_n)) = \mathbf{P}(-C^{-1}H \in \{u : \varphi^*(Cu) \le \eta_\alpha\})
$$

$$
= \mathbf{P}(\varphi^*(H) \le \eta) = 1 - \alpha.
$$

where  $\eta_\alpha$  is the  $(1-\alpha)$ -quantile of the random variable  $\varphi^*(\mathcal{H}).$ 

## Approximation of confidence regions

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$$
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$$

 $\Lambda_{\delta_n}(P_n)$  is generally challenging to compute. Here we provide an approximation of  $\Lambda_{\delta_n}(P_n)$  based on the following corollary.

Corollary (informal)

Under the assumptions of main theorem, we have (omitting  $\gamma$  in  $\Lambda_{n,\gamma}$ )

$$
\Lambda_{\delta_n}(P_n) \approx \beta_n^{ERM} + n^{-1/2} \Lambda_n \approx \beta_n^{ERM} + n^{-1/2} \Lambda_n^n.
$$

where  $\Lambda_\eta^n:=\{u:\varphi_n^*(C_nu)\leq\eta\}$  and  $\varphi_n(\cdot),$   $C_n$  are the empirical analogs of  $\varphi(\cdot), C$ .

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Evaluating convex conjugate is generally time-consuming. We give a computationally efficient algorithm of  $\Lambda_n$  using support function.

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```
- Evaluating convex conjugate is generally time-consuming. We give a computationally efficient algorithm of  $\Lambda_n$  using support function.
- For any  $u_1,...,u_m\in\mathbb{R}^d,$  with  $\|u_i\|_2=1$  we have

$$
\Lambda_{\eta}=\cap_{u}\lbrace v: u\cdot v\leq h_{\Lambda_{\eta}}(u)\rbrace\subset \cap_{u_1,...u_m}\lbrace v: u_i\cdot v\leq h_{\Lambda_{\eta}}(u_i)\rbrace.
$$

We can sample directions  $u_1, ..., u_m$  to obtain a tight envelope of  $\Lambda_n$ .

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We can sample directions  $u_1, ..., u_m$  to obtain a tight envelope of  $\Lambda_n$ .  $\mathcal{h}_{\mathsf{\Lambda}_{\eta}}(\mathsf{v})$  is the support function of the convex set  $\mathsf{\Lambda}_{\eta},$  defined as

$$
h_{\Lambda_{\eta}}(x) := \sup_{a} \{x \cdot a : a \in \Lambda_{\eta}\} = 2\sqrt{\eta \varphi(C^{-1}v)},
$$

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h_{\Lambda_{\eta}}(x) := \sup_{a} \{x \cdot a : a \in \Lambda_{\eta}\} = 2\sqrt{\eta \varphi(C^{-1}v)},
$$

A completely analogous method can be used to estimate  $\Lambda_{\eta}^n.$ 

## Confidence regions of square-root LASSO



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Figure: Confidence regions for different norms centered at the ERM solution<br>
confidence Regions in DRO (Conformer 24, 2019) [Confidence Regions in DRO](#page-0-0) 0ctober 24, 2019 19 / 21

### **Contributions**

<span id="page-32-0"></span>

- Asymptotic normality of Wasserstein-DRO estimators: arbitrary scaling of uncertainty size.
- Suitable confidence regions for DRO problems: coverage, approximation and computation.





Blanchet, J., Murthy, K., & Si, N. (2019). Confidence Regions in Wasserstein Distributionally Robust Estimation. arXiv preprint arXiv:1906.01614.

# <span id="page-33-0"></span>Thanks!