Data-driven Sample Average Approximation with Covariate Information

Güzin Bayraksan

Department of Integrated Systems Engineering
The Ohio State University

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Rohit Kannan
Los Alamos National Lab

Jim Luedtke
University of Wisconsin-Madison

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Outline

1. Introduction and Motivation

2. Empirical Residuals SAA
   - Theoretical Analysis
   - Computational Results

3. Distributionally Robust ER-SAA
   - Theoretical Analysis
   - Computational Results

4. Conclusions and Future Work
Traditional Stochastic Programs

- Traditional Stochastic Programs consider

\[
\min_{z \in \mathcal{Z}} \mathbb{E} [c(z, Y)],
\]

where
- \( Y \) denotes the uncertain model parameters (a random vector),
- \( \mathcal{Z} \) denotes the feasible region for decisions \( z \).
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where

- $Y$ denotes the uncertain model parameters (a random vector),
- $\mathcal{Z}$ denotes the feasible region for decisions $z$.

Suppose we have access to (i.i.d.) observations $\{y^i\}_{i=1}^n$ of $Y$. 

SAA framework has well established theory: consistency, rates of convergence, ... (Shapiro et al., 2009) (Homem-de Mello and Bayraksan, 2014)
Traditional Stochastic Programs

- Traditional Stochastic Programs consider

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  where
  - \( Y \) denotes the uncertain model parameters (a random vector),
  - \( \mathcal{Z} \) denotes the feasible region for decisions \( z \).

- Suppose we have access to (i.i.d.) observations \( \{y^i\}_{i=1}^n \) of \( Y \).

- Then, the **Sample Average Approximation (SAA)** is given by

  \[ \min_{z \in \mathcal{Z}} \frac{1}{n} \sum_{i=1}^{n} c(z, y^i). \]

SAA framework has well established theory: consistency, rates of convergence, \( \ldots \) (Shapiro et al., 2009) (Homem-de Mello and Bayraksan, 2014)
Given a covariate realization $X = x$, update the Stochastic Program to

$$\min_{z \in Z} \mathbb{E} [c(z, Y) \mid X = x].$$

(\text{SP})

Covariates are also known as side information, or auxiliary variables, or features

(Bertsimas and Kallus, 2019)
Example Applications

**Portfolio Optimization**  
(Bazier-Matte and Delage, 2020)

- **Y**: Return of stocks
- **X**: Market indicators; Company data
- **z**: Portfolio decisions

**Power Grid Scheduling**  
(Donti et al., 2017)

- **Y**: Load; Renewal Energy Outputs
- **X**: Weather forecast; Time/Day
- **z**: Generator scheduling decisions
Suppose we have data of form (not necessarily i.i.d.)

$$\mathcal{D}_n := \{(y^i, x^i)\}_{i=1}^n$$

(uncertain parameters, and covariates)
How to Form SAA with Covariate Information?

- Suppose we have data of form (not necessarily i.i.d.)

\[ D_n := \{(y^i, x^i)\}_{i=1}^n \]

(uncertain parameters, and covariates)

- When making decision \( z \), we observe a **new** covariate \( x \)
How to Form SAA with Covariate Information?

- Suppose we have data of form (not necessarily i.i.d.)
  \[ D_n := \{(y^i, x^i)\}_{i=1}^n \]
  (uncertain parameters, and covariates)

- When making decision \( z \), we observe a new covariate \( x \)

- How can we form SAA with this data? Two Components:
  1. “Learn” — Predict \( Y \) given \( X = x \)
  2. “Optimize” — Integrate Learning into Optimization (with errors)
Integrated Learning and Optimization

**Approach 1: Empirical Risk Minimization (ERM) [Solution Learning]**

- Attempt to directly learn a mapping from $x$ to a solution $z$ (Bertsimas and Kallus (2019); Ban and Rudin (2018))
- Handling constraints and large dimensions of $z$ is challenging

**Approach 2: Modify the Optimization Step (this work)**

Change optimization model to reflect uncertainty in prediction (Ban et al. (2018), Sen and Deng (2018), Bertsimas and Kallus (2019))

**Approach 3: Modify the Learning Step**

Change loss function in training step to reflect use of prediction in optimization model (Donti et al. (2017), Elmachtoub and Grigas (2021))

Results in a challenging training problem; Can be less modular but lower cost
Integrated Learning and Optimization

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Introduction and Motivation

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“True” Relationship Between $Y$ and $X$

Assume

$$Y|\{X = x\} = f^*(x) + \varepsilon,$$

where

- $f^*(x) := \mathbb{E}[Y \mid X = x]$ is the regression function
- $f^*$ belongs to a known class of functions $\mathcal{F}$ (can be infinite dimensional or depend on $n$)
- $\varepsilon$ is the associated regression error
- $\varepsilon$ are independent of the covariates $X$
- $\mathbb{E}[\varepsilon] = 0$
“True” Stochastic Program and SAA

Under this structure, the “true” conditional stochastic program (SP) is equivalent to

$$\min_{z \in \mathcal{Z}} \mathbb{E} [c(z, Y) \mid X = x]$$  (1)
“True” Stochastic Program and SAA

Under this structure, the “true” conditional stochastic program (SP) is equivalent to

$$\min_{z \in Z} \mathbb{E} [c(z, f^*(x) + \varepsilon)]$$  \hspace{1cm} (1)
“True” Stochastic Program and SAA

- Under this structure, the “true” conditional stochastic program (SP) is equivalent to

\[
\min_{z \in \mathcal{Z}} \mathbb{E} [c(z, f^*(x) + \varepsilon)] \tag{1}
\]

- Given data \( \mathcal{D}_n := \{(y^i, x^i)\}_{i=1}^n \) (not necessarily i.i.d.) and errors

\[
\varepsilon^i := y^i - f^*(x^i), \quad \forall i \in \{1, \cdots, n\}
\]

- We can form Full-Information SAA

\[
\min_{z \in \mathcal{Z}} \frac{1}{n} \sum_{i=1}^n c(z, f^*(x) + \varepsilon^i) \tag{2}
\]
“True” Stochastic Program and SAA

Under this structure, the “true” conditional stochastic program (SP) is equivalent to

\[
\min_{z \in Z} \mathbb{E} [c(z, f^*(x) + \varepsilon)]
\] (1)

Given data \( D_n := \{(y^i, x^i)\}_{i=1}^n \) (not necessarily i.i.d.) and errors

\[\varepsilon^i := y^i - f^*(x^i), \quad \forall i \in \{1, \ldots, n\}\]

We can form Full-Information SAA

\[
\min_{z \in Z} \frac{1}{n} \sum_{i=1}^n c(z, f^*(x) + \varepsilon^i)
\] (2)
Empirical Residuals-Based SAA

Approach suggested by Sen and Deng (2018) and Ban et al. (2018) is

1. **Estimate** $f^*$ **using your favorite Statistical / Machine Learning (ML) model** \( \Rightarrow \hat{f}_n \)

*Example:*

\[
\hat{f}_n(\cdot) \in \arg\min_{f(\cdot) \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \ell \left( y^i, f(x^i) \right)
\]

with some loss function \( \ell : \mathbb{R}^{d_y} \times \mathbb{R}^{d_y} \rightarrow \mathbb{R}_+ \)
2. **Compute empirical residuals**

\[ \hat{\varepsilon}_n^i := y^i - \hat{f}_n(x^i), \quad i = 1, \ldots, n \]

3. **Use** \( \{ \hat{f}_n(x) + \hat{\varepsilon}_n^i \}_{i=1}^n \) **as proxy** for samples of \( Y \) given \( X = x \)

\[
\min_{z \in \mathcal{Z}} \frac{1}{n} \sum_{i=1}^n c(z, \hat{f}_n(x) + \hat{\varepsilon}_n^i) \tag{ER-SAA}
\]
Empirical Residuals-Based SAA

2. Compute empirical residuals

\[ \hat{\epsilon}_n^i := y^i - \hat{f}_n(x^i), \quad i = 1, \ldots, n \]

3. Use \( \{ \hat{f}_n(x) + \hat{\epsilon}_n^i \}_{i=1}^n \) as proxy for samples of \( Y \) given \( X = x \)

\[
\min_{z \in \mathcal{Z}} \frac{1}{n} \sum_{i=1}^{n} c(z, \hat{f}_n(x) + \hat{\epsilon}_n^i) \quad \text{(ER-SAA)}
\]

- General analysis
- Improvements when sample size is small?
Theoretical Analysis of ER-SAA
Sequence of Problems & Notation

- **“True” conditional stochastic program**

\[
v^*(x) := \min_{z \in Z} \left\{ g(z; x) := \mathbb{E} [c(z, f^*(x) + \varepsilon)] \right\}
\]  \hspace{1cm} (3)

- **Full-Information SAA**

\[
\min_{z \in Z} \left\{ g_n^*(z; x) := \frac{1}{n} \sum_{i=1}^{n} c(z, f^*(x) + \varepsilon^i) \right\}
\]  \hspace{1cm} (4)

- **Empirical Residuals-Based SAA (ER-SAA)**

\[
\hat{\nu}_n^{ER}(x) := \min_{z \in Z} \left\{ \hat{g}_n^{ER}(z; x) := \frac{1}{n} \sum_{i=1}^{n} c \left( z, \hat{f}_n(x) + \varepsilon_n^i \right) \right\}
\]  \hspace{1cm} (5)
Sequence of Problems & Notation

- **“True” conditional stochastic program**

\[
\nu^*(x) := \min_{z \in Z} \left\{ g(z; x) := \mathbb{E} [c(z, f^*(x) + \varepsilon)] \right\}
\]  

(3)

- **Full-Information SAA**

\[
\min_{z \in Z} \left\{ g^*_n(z; x) := \frac{1}{n} \sum_{i=1}^{n} c(z, f^*(x) + \varepsilon^i) \right\}
\]  

(4)

- **Empirical Residuals-Based SAA (ER-SAA)**

\[
\hat{\nu}^{ER}_n(x) := \min_{z \in Z} \left\{ \hat{g}^{ER}_n(z; x) := \frac{1}{n} \sum_{i=1}^{n} c \left( z, \hat{f}_n(x) + \hat{\varepsilon}_n^i \right) \right\}
\]  

(5)
Notation regarding optimal solutions

- $S^*(x)$ — set of optimal solutions to “true” problem
- $\hat{z}_{ER}^n(x) \in \hat{S}^{ER}_n(x)$ — an optimal solution $\in$ set of optimal solutions to (ER-SAA)

Assume $S^*(x)$ and $\hat{S}^{ER}_n(x)$ are nonempty for almost every (a.e.) $x \in \mathcal{X}$
Consistency and Asymptotic Optimality:
Assumption on Problem Structure

Assumption

For each $z \in \mathcal{Z}$, the function $c$ in problem (3) satisfies the **Lipschitz condition**

$$|c(z, y) - c(z, \bar{y})| \leq L(z)\|\bar{y} - y\|, \quad \forall y, \bar{y} \in \mathbb{R}^{d_y},$$

with Lipschitz constant $L$ satisfying $\sup_{z \in \mathcal{Z}} L(z) < +\infty$.

Can be Satisfied by Two-Stage Stochastic Linear Programs

Note: This assumption can be relaxed to local Lipschitz continuity with additional conditions on the regression step
Consistency and Asymptotic Optimality:

Assumption on Uniform Convergence of Full-Information SAA Objective Functions to True Problem Objective Function

**Assumption**

For a.e. $x \in \mathcal{X}$, the sequence of sample average functions $\{g^*_n(\cdot; x)\}$ defined in (4) **converges in probability to the true function $g(\cdot; x)$** defined in (3) **uniformly** on the set $\mathcal{Z}$.

Follows under conditions stipulated in classical SAA analysis.
Consistency and Asymptotic Optimality:
Assumption on Learning Step

Assumption

The regression/learning procedure satisfies the following consistency properties:

1. **Pointwise error consistency**: $\hat{f}_n(x) \xrightarrow{p} f^*(x)$ for a.e. $x \in \mathcal{X}$,

2. **Mean-squared estimation error consistency**: 

$$\frac{1}{n} \sum_{i=1}^{n} \| f^*(x^i) - \hat{f}_n(x^i) \|^2 \xrightarrow{p} 0,$$

where $\xrightarrow{p}$ denotes convergence in probability.

Can hold under appropriate conditions for Ordinary Least Squares (OLS), $k$ Nearest Neighbor (kNN) regression, and Random Forests (RF), ...
Consistency and Asymptotic Optimality

Theorem

Under the above assumptions, we have

1. \( \hat{v}_n^{ER}(x) \xrightarrow{p} v^*(x), \)

2. \( \mathbb{D} \left( \hat{S}_n^{ER}(x), S^*(x) \right) \xrightarrow{p} 0, \) and

3. \( \sup_{z \in \hat{S}_n^{ER}(x)} g(z; x) \xrightarrow{p} v^*(x) \) for a.e. \( x \in \mathcal{X}, \)

where \( \xrightarrow{p} \) denotes convergence in probability, and for sets \( A, B \subseteq \mathbb{R}^{d_z}, \) let \( \mathbb{D}(A, B) := \sup_{v \in A} \text{dist}(v, B) \) denote the deviation of \( A \) from \( B, \) where \( \text{dist}(v, B) := \inf_{w \in B} \| v - w \|. \)
Rates of Convergence

Similar results can be obtained on rate of convergence by strengthening the assumptions.

Assumption
There is a constant $0 < \alpha \leq 1$ (that is independent of the number of samples $n$, but could depend on the dimension $d_x$ of the covariates $X$) such that the regression procedure satisfies the following asymptotic convergence rate criteria:

1. Pointwise error rate:
   \[
   \|f^*(x) - \hat{f}_n(x)\|^2 = O_p(n^{-\alpha}) \text{ for a.e. } x \in X,
   \]

2. Mean-squared estimation error rate:
   \[
   \frac{1}{n} \sum_{i=1}^{n} \|f^*(x_i) - \hat{f}_n(x_i)\|^2 = O_p(n^{-\alpha}).
   \]

OLS, Lasso satisfy assumption with $\alpha = 1$
KNN, RF satisfy assumption with $\alpha = O(1)$

Kannan, Luedtke & Bayraksan
Rates of Convergence

Similar results can be obtained on rate of convergence by strengthening the assumptions

Assumption

There is a constant $0 < \alpha \leq 1$ (that is independent of the number of samples $n$, but could depend on the dimension $d_x$ of the covariates $X$) such that the regression procedure satisfies the following asymptotic convergence rate criteria:

1. **Pointwise error rate**: $\|f^*(x) - \hat{f}_n(x)\|^2 = O_p(n^{-\alpha})$ for a.e. $x \in \mathcal{X}$,

2. **Mean-squared estimation error rate**: $\frac{1}{n} \sum_{i=1}^{n} \|f^*(x_i) - \hat{f}_n(x_i)\|^2 = O_p(n^{-\alpha})$. 
Rates of Convergence

Similar results can be obtained on rate of convergence by strengthening the assumptions

Assumption

There is a constant $0 < \alpha \leq 1$ (that is independent of the number of samples $n$, but could depend on the dimension $d_x$ of the covariates $X$) such that the regression procedure satisfies the following asymptotic convergence rate criteria:

1. **Pointwise error rate**: \[ \| f^*(x) - \hat{f}_n(x) \|^2 = O_p(n^{-\alpha}) \text{ for a.e. } x \in \mathcal{X}, \]

2. **Mean-squared estimation error rate**: \[ \frac{1}{n} \sum_{i=1}^{n} \| f^*(x^i) - \hat{f}_n(x^i) \|^2 = O_p(n^{-\alpha}). \]

OLS, Lasso satisfy assumption with $\alpha = 1$ 

kNN, RF satisfy assumption with $\alpha = \frac{O(1)}{d_x}$
Theorem

Under the above assumptions, plus continuity assumptions and a functional Central Limit Theorem assumption, we have

$$\hat{v}_n^{ER}(x) = v^*(x) + \tilde{o}_p(n^{-\alpha/2}) \quad \text{for a.e. } x \in \mathcal{X},$$

where $\tilde{o}$ notation hides polylogarithmic factors in $n$.
Finite Sample Guarantees

- \( \kappa > 0 \): optimality gap, \( \delta \in (0, 1) \): reliability level

Recall that
- \( \hat{S}^{ER}_n(x) \) — set of optimal solutions to ER-SAA at covariate value \( x \)
- \( S^\kappa(x) \) — set of \( \kappa \)-optimal solutions to the “True” problem at \( x \)

Estimate sample size \( n \) required for

\[
P \left\{ \hat{S}^{ER}_n(x) \subseteq S^\kappa(x) \right\} \geq 1 - \delta,
\]

i.e., optimal solutions of ER-SAA approximation are \( \kappa \)-optimal to the true problem with probability \( \geq 1 - \delta \)
Finite Sample Guarantees

Two effects:

1. Sample size required for “Full-Information” SAA to be close to “True” Problem

\[ n \geq \frac{O(1)\sigma_c^2(x)}{\kappa^2} \left[ d_x \log \left( \frac{O(1)D}{\kappa} \right) + \log \left( \frac{O(1)}{\delta} \right) \right] \]

from classical SAA analysis.

2. Sample size required for ER-SAA to be close to “Full-Information” SAA

[Note: For brevity, some variance terms are omitted throughout this section]
Finite Sample Guarantees

- If $f^*$ is linear and we use OLS regression, then holds if
  \[ n \geq N_C + \frac{O(1)}{\kappa^2 d_y} \left[ \log \left( \frac{O(1)}{\delta} \right) + d_x \right] \]

- If $f^*$ is $s$-sparse linear and we use the Lasso, then holds if
  \[ n \geq N_C + \frac{O(1)}{\kappa^2 d_y} \left[ s \log \left( \frac{O(1)}{\delta} \right) + s \log(d_x) \right] \]
Finite Sample Guarantees

- If $f^*$ is \textbf{Lipschitz continuous} and we use \textbf{kNN} regression with $k = \lceil O(1) n^\gamma \rceil$ for some constant $\gamma \in (0, 1)$, then holds if

$$n \geq N_C + \left( \frac{O(1) d_y}{\kappa^2} \right)^{\frac{1}{\gamma}} \left[ d_x \log \left( \frac{O(1)}{d_x} \right) + \log \left( \frac{O(1)}{\delta} \right) \right]^{\frac{1}{\gamma}}$$

$$+ \left( \frac{O(1) d_y}{\kappa^2} \right)^{d_x} \left[ \frac{d_x}{2} \log \left( \frac{O(1) d_x d_y}{\kappa^2} \right) + \log \left( \frac{O(1)}{\delta} \right) \right]$$
Finite Sample Guarantees: What does it all mean?

- **Prediction** of the regression function \( f^* \) introduces additional terms that depend on the dimensions \( d_y \) and \( d_x \) of the random vector \( Y \) and the covariates \( X \).

- Assuming that the regression function \( f^* \) satisfies the necessary structural properties, using **OLS regression or the Lasso** for the regression step can yield sample size estimates that **depend modestly** on the accuracy \( \kappa \) and the dimensions \( d_x \) and \( d_y \).

- The sample size estimates for **kNN regression** are valid under mild assumptions on the regression function \( f^* \), but more heavily dependent on \( d_x \) and \( d_y \).
Computational Results on ER-SAA
Two-Stage Resource Allocation Model (Luedtke, 2014)

- Meet demands of $|\mathcal{J}| = 30$ customers using 20 resources

- Uncertain demands $Y$ generated according to

$$Y_j = \varphi_j^* + \sum_{l \in \mathcal{L}^*} \zeta_j^* \cdot (X_l)^\theta + \varepsilon_j, \quad \forall j \in \mathcal{J},$$

where

- $\theta \in \{0.5, 1, 2\}$ is a fixed parameter that determines the model class,
- $\varepsilon_j \sim \mathcal{N}(0, \sigma_j^2)$ is an additive error, and
- Covariate dimension $d_x \in \{3, 10, 100\}$
- $|\mathcal{L}^*| = 3$, i.e., the demands truly depend only on 3 covariates
Computational Setup

- Fit **linear** model with OLS/Lasso regression (even when $\theta \neq 1$)

  \[
  Y_j = \varphi_j + \sum_{l \in L} \zeta_{jl} \cdot X_l + \eta_j, \quad \forall j \in J,
  \]

  where $\eta_j$ are zero-mean errors, using OLS or Lasso regression

- Estimate optimality gap of solutions $\hat{z}^{ER}_n(x)$

  \[
  \hat{z}^{ER}_n(x) \in \arg \min_{z \in \mathbb{Z}} \frac{1}{n} \sum_{i=1}^{n} c(z, \hat{f}_n(x) + \tilde{\varepsilon}_n)
  \]
Effect of Varying Covariate Dimension:

with correct ($\theta = 1$) or incorrect ($\theta \neq 1$) regression fit
Results with correct model class ($\theta = 1$)

Red (E): ER-SAA + OLS
Black (k): Reweighted SAA with kNN (Bertsimas and Kallus, 2019)

Boxes: 25 and 75 percentiles of Upper Confidence Bounds (UCB)
Whiskers: 2 and 98 percentiles
Results with misspecified model class ($\theta \neq 1$)

$p = 0.5$

$p = 2$
Effect of Prediction Model:

with correct ($\theta = 1$) or incorrect ($\theta \neq 1$) regression fit
Effect of Prediction Model ($\theta = 1$)

Red (E): ER-SAA + OLS
Blue(L): ER-SAA + Lasso

![Box plots showing the effect of prediction model on % optimality gap.](image-url)
Effect of Prediction Model with misspecified model ($\theta \neq 1$)

$p = 0.5$

$p = 2$
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Empirical Residuals-Based DRO

DRO can regularize small-sample ER-SAA, yielding solutions with better out-of-sample performance.
Empirical Residuals-Based DRO

DRO can regularize small-sample ER-SAA, yielding solutions with better out-of-sample performance

Given “estimated” empirical distribution

\[
\hat{P}_n^{ER}(x) := \frac{1}{n} \sum_{i=1}^{n} \delta_{\hat{f}_n(x) + \xi_i},
\]

Consider Empirical Residuals-Based DRO

\[
\min_{z \in Z} \max_{Q \in \hat{P}_n(x)} \mathbb{E}_{Y \sim Q}[c(z, Y)],
\]

where \(\hat{P}_n(x)\) is an ambiguity set containing \(\hat{P}_n^{ER}(x)\)
How to Form the Ambiguity Set $\hat{\mathcal{P}}_n(x)$

Let $\mathcal{Y} \subseteq \mathbb{R}^{d_y}$ denote the support of $Y$

1. **Wasserstein-$p$, $p \in [1, +\infty]$** (Esfahani and Kuhn, 2018)

$$\hat{\mathcal{P}}_n(x) = \{ Q \in \mathcal{P}(\mathcal{Y}) : d_{W,p}(Q, \hat{\mathcal{P}}_{n\text{ER}}(x)) \leq \zeta_n(x) \}.$$
How to Form the Ambiguity Set $\hat{P}_n(x)$

Let $\mathcal{Y} \subseteq \mathbb{R}^{d_Y}$ denote the support of $Y$

1. **Wasserstein-$p$, $p \in [1, +\infty]$** (Esfahani and Kuhn, 2018)

   \[ \hat{P}_n(x) = \left\{ Q \in \mathcal{P}(\mathcal{Y}) : d_{W,p}(Q, \hat{P}_{nER}^{ER}(x)) \leq \zeta_n(x) \right\}. \]

2. **Sample-robust** (Bertsimas, Shtern, and Sturt, 2018)

   \[ \hat{P}_n(x) = \left\{ Q = \frac{1}{n} \sum_{i=1}^{n} \delta_{\bar{y}^i} : \| \bar{y}^i - (\hat{f}_n(x) + \hat{\epsilon}_n) \| \leq \mu_n(x), \bar{y}^i \in \mathcal{Y}, \forall i \right\}. \]
How to Form the Ambiguity Set $\hat{P}_n(x)$

Let $Y \subseteq \mathbb{R}^{d_y}$ denote the support of $Y$

1. **Wasserstein-$p$, $p \in [1, +\infty]$** (Esfahani and Kuhn, 2018)

   $$\hat{P}_n(x) = \left\{ Q \in \mathcal{P}(Y) : d_{W,p}(Q, \hat{P}_n^{ER}(x)) \leq \zeta_n(x) \right\}.$$

2. **Sample-robust** (Bertsimas, Shtern, and Sturt, 2018)

   $$\hat{P}_n(x) = \left\{ Q = \frac{1}{n} \sum_{i=1}^{n} \delta_{\bar{y}^i} : \|\bar{y}^i - (\hat{f}_n(x) + \hat{\varepsilon}_n^i)\| \leq \mu_n(x), \bar{y}^i \in Y, \forall i \right\}.$$

3. **$\phi$-Divergence (or other) with the same support as $\hat{P}_n^{ER}(x)$**
   
   Kullback-Leibler divergence, Variation distance, Hellinger distance, ...
Some Theoretical Results on DRO-ER-SAA
Preliminaries

Let us focus on \textit{Wasserstein-}p, \( p \in [1, +\infty) \)

Given \( Q_1, Q_2 \in \mathcal{P}(S) \), let \( \Pi(Q_1, Q_2) \) denote the set of joint distributions with marginals \( Q_1 \) and \( Q_2 \). The \( p \)-Wasserstein distance \( d_{W,p}(Q_1, Q_2) \) between \( Q_1 \) and \( Q_2 \) with respect to the \( \ell_2 \)-norm \( \| \cdot \| \) is given by

\[
d_{W,p}(Q_1, Q_2) := \left( \inf_{\pi \in \Pi(Q_1, Q_2)} \int_S \|y_1 - y_2\|^p d\pi(y_1, y_2) \right)^{1/p}
\]

\(^1\)Our results can be extended to Wasserstein distances defined using \( \ell_q \)-norms with \( q \neq 2 \).
Optimal value

\[
\hat{v}^{DRO}_n(x) = \min_{z \in \mathcal{Z}} \sup_{Q \in \hat{\mathcal{P}}_n(x)} E_{Y \sim Q}[c(z, Y)],
\]

Optimal solution

\[
\hat{z}^{DRO}_n(x) \in \arg \min_{z \in \mathcal{Z}} \sup_{Q \in \hat{\mathcal{P}}_n(x)} E_{Y \sim Q}[c(z, Y)].
\]

**Note:** Some details will be skipped for brevity. For precise statements, please see arXiv:2012.01088
Toward Convergence Theory for Wasserstein ER-DRO

**Assumption:** For any risk level $\alpha \in (0, 1)$, there exists a constant $\kappa_{p,n}(\alpha, x) > 0$ such that the regression procedure satisfies

$$
\mathbb{P}\left\{ \| f^*(x) - \hat{f}_n(x) \|^p > \kappa_{p,n}^p(\alpha, x) \right\} \leq \alpha, \quad \text{and}
$$

$$
\mathbb{P}\left\{ \frac{1}{n} \sum_{i=1}^{n} \| f^*(x^i) - \hat{f}_n(x^i) \|^p > \kappa_{p,n}^p(\alpha, x) \right\} \leq \alpha.
$$
Toward Convergence Theory for Wasserstein ER-DRO

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Holds for Wasserstein order $p = 2$ and

- **OLS, Lasso** with $\kappa_{2,n}^2(\alpha, x) = O(n^{-1} \log(\alpha^{-1}))$
- **CART, RF** with $\kappa_{2,n}^2(\alpha, x) = O(n^{-1} \log(\alpha^{-1}))^{O(1)/d_x}$
Given covariate realization $x$ and risk level $\alpha \in (0, 1)$, use

$$\zeta_n(\alpha, x) := 2\kappa_{p,n}(\alpha/4, x) + \bar{\kappa}_{p,n}(\alpha/2)$$

as the radius of the Wasserstein ambiguity set, where

$$\bar{\kappa}_{p,n}(\alpha/2) = \text{traditional Wasserstein DRO radius that is used if we know } f^* \text{ (Kuhn et al., 2019)}$$

**Note:** Radius guarantees

$$\mathbb{P}\left\{ d_W(\hat{P}_n^{ER}(x), P_Y|X=x) > \zeta_n(\alpha, x) \right\} \leq \alpha$$
Wasserstein ER-DRO Results: Finite Sample Certificate Guarantee

The optimal value $\hat{v}_{n}^{DRO}(x)$ provides the following certificate on the out-of-sample cost of $\hat{z}_{n}^{DRO}(x)$:

"Informal" Theorem [Finite Sample Certificate Guarantee]

For the above choice of the Wasserstein radius $\zeta_{n}(\alpha, x)$, under appropriate conditions, the solution $\hat{z}_{n}^{DRO}(x)$ and the optimal value $\hat{v}_{n}^{DRO}(x)$ satisfy

$$\mathbb{P} \left\{ \mathbb{E}_{\varepsilon} \left[ c(\hat{z}_{n}^{DRO}(x), f^{*}(x) + \varepsilon) \right] \leq \hat{v}_{n}^{DRO}(x) \right\} \geq 1 - \alpha$$
Wasserstein ER-DRO Results: Rate of Convergence

“Informal” Theorem [Rate of Convergence]

Suppose there is a sequence of risk levels \( \{\alpha_n\} \subset (0, 1) \) such that \( \sum_n \alpha_n < +\infty \) and the radius satisfies \( \lim_{n \to \infty} \zeta_n(\alpha_n, x) = 0 \). Then, under appropriate assumptions, the sequence \( \{\hat{z}_n^{DRO}(x)\} \) of solutions satisfies

\[
\hat{v}_n^{DRO}(x) = v^*(x) + O_p(\zeta_n(\alpha_n, x))
\]

\[
\mathbb{E}_\varepsilon \left[ c(\hat{z}_n^{DRO}(x), f^*(x) + \varepsilon) \right] = v^*(x) + O_p(\zeta_n(\alpha_n, x))
\]

where \( v^*(x) \) is the optimal value of the true conditional stochastic program (SP).
Choosing the Wasserstein Radius in Practice

- Theoretical Wasserstein radius: involves unknown constants and is typically conservative

- **Use cross-validation** to specify the radius $\zeta_n(x)$
  - **Approach 1**: Ignore covariate information altogether while choosing $\zeta_n$
  - **Approach 2**: Use the data $D_n$ (including covariates) to choose $\zeta_n$ independently of the new covariate realization $X = x$
  - **Approach 3**: Use both the data $D_n$ and the new covariate realization $X = x$ to choose the radius $\zeta_n(x)$

- Approach 3 is more data intensive than Approaches 1 & 2
Computational Results on DRO-ER-SAA
Numerical Study: Mean-Risk Portfolio Optimization

\[
\min_{z \in \mathcal{Z}} \mathbb{E}_{Y}[ -Y^T z ] + \rho \text{CVaR}_\beta(-Y^T z),
\]

where \( \mathcal{Z} := \{ z \in \mathbb{R}_+^{d_Z} : \sum_i z_i = 1 \} \).

- \( z_i \): fraction of capital invested in asset \( i \)
- \( Y_i \): uncertain net return of asset \( i \)
- \( \text{CVaR}_\beta \approx \) average of the \( 100(1 - \beta)\% \) worst return outcomes
- \( \rho \geq 0 \) and \( \beta \in [0, 1) \): risk parameters (e.g., \( \rho = 10, \beta = 0.8 \))
Numerical Study: Mean-Risk Portfolio Optimization

- Consider instance with 10 assets
- Uncertain returns $Y$ generated according to

$$Y_j = \nu^*_j + \sum_{l=1}^{3} \mu^*_j(X_l)^\theta + \bar{\epsilon}_j + \omega, \quad \forall j \in \{1, \ldots, 10\},$$

where $\bar{\epsilon}_j \sim \mathcal{N}(0, 0.02j)$, $\omega \sim \mathcal{N}(0, 0.02)$, $\theta \in \{0.5, 1, 2\}$,
$\dim(X) \in \{10, 100\}$.
Numerical Study: Mean-Risk Portfolio Optimization

- Consider instance with 10 assets
- Uncertain returns \( Y \) generated according to

\[
Y_j = \nu_j^* + \sum_{l=1}^{3} \mu_{jl}^* (X_l)^{\theta} + \bar{\varepsilon}_j + \omega, \quad \forall j \in \{1, \ldots, 10\},
\]

where \( \bar{\varepsilon}_j \sim \mathcal{N}(0, 0.02j) \), \( \omega \sim \mathcal{N}(0, 0.02) \), \( \theta \in \{0.5, 1, 2\} \), \( \text{dim}(X) \in \{10, 100\} \)

- Fit linear model with OLS/Lasso regression (even when \( \theta \neq 1 \))

\[
Y_j = \nu_j + \sum_{l=1}^{\text{dim}(X)} \mu_{jl} X_l + \eta_j, \quad \forall j \in \{1, \ldots, 10\},
\]

where \( \eta_j \) are zero-mean errors

- Estimate optimality gap of solutions \( \hat{z}_{n}^{ER}(x) \) and \( \hat{z}_{n}^{DRO}(x) \)
Results with OLS and Correct Model Class ($\theta = 1$)

$I^*$: Ideal Wasserstein radius (only for benchmarking)

1 & 2: Wasserstein radius specified using Approaches 1 & 2

E: ER-SAA + OLS

Lower y-axis value $\implies$ closer to optimal

Boxes: 25, 50, and 75 percentiles of upper confidence bounds

Whiskers: 2 and 98 percentiles

Sample sizes: $\{1.5, 2, 3, 5\} \times (\text{dim}(X) + 1)$
Results with OLS and Misspecified Model Class ($\theta \neq 1$)

**$\theta = 0.5$**

- $d_x = 10$
- $d_x = 100$

**$\theta = 2$**

- $d_x = 10$
- $d_x = 100$
Modularity Benefit for $d_x = 100$: Bring on Lasso

$W$: Wasserstein radius for ER-DRO + Lasso using Approach 2

$E$: ER-SAA + Lasso

Lower y-axis value $\implies$ closer to optimal

Boxes: 25, 50, and 75 percentiles of upper confidence bounds
Whiskers: 2 and 98 percentiles

Sample sizes: $\{0.5, 0.8, 1.2, 1.5\} \times (\text{dim}(X) + 1)$
Outline

1. Introduction and Motivation

2. Empirical Residuals SAA
   ▶ Theoretical Analysis
   ▶ Computational Results

3. Distributionally Robust ER-SAA
   ▶ Theoretical Analysis
   ▶ Computational Results

4. Conclusions and Future Work
Extension: Handling Heteroscedastic Errors

(arXiv:2101.03139)

- **Assumption thus far:** true model is $Y = f^*(X) + \varepsilon$ with errors $\varepsilon$ independent of covariates $X$

- **Assumption may be violated for some applications**
  - Example: variability of product demands/wind generators can depend on seasonality/location

- **Relaxed assumption:** $Y = f^*(X) + Q^*(X)\varepsilon$ with $X$, $\varepsilon$ independent
  - Estimate $f^*$ and $Q^*$ $\implies$ estimate samples of $\varepsilon$
  - Theoretical results for ER-SAA and ER-DRO readily generalize

Thanks to Erick Delage
Concluding Remarks

Empirical residuals formulations: A modular approach to using covariate information in optimization

- Converges under appropriate assumptions on prediction and optimization models
- Trade-off in choosing prediction model class: using a misspecified model can lead to better results with limited data
- DRO variant outperforms with limited data, benefit diminishes with increased data
Concluding Remarks

Empirical residuals formulations: A modular approach to using covariate information in optimization

- Converges under appropriate assumptions on prediction and optimization models
- Trade-off in choosing prediction model class: using a misspecified model can lead to better results with limited data
- DRO variant outperforms with limited data, benefit diminishes with increased data

Future research directions

- Formulations with stochastic constraints, discrete recourse decisions; robust multistage optimization
- Application to energy systems optimization
Thank you!

(bayraksan.1@osu.edu)

Preprints available at

ER-SAA:
http://www.optimization-online.org/DB_FILE/2020/07/7932.pdf

DRO-ER-SAA:


