Learning-Assisted Data-Driven Optimization

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Outline

1. Research Overview
2. Stochastic Programming with Covariate Information
3. Learning to Accelerate the Global Optimization of QCQPs
Research Overview

- Accelerating Global Optimization
- Flexible Energy Polygeneration
- Integrating Renewables in the Grid
- Modeling Grid Resilience
- Accelerating Global Optimization
- Branch & Bound Complexity Analysis
- Decomposition Methods for Stochastic MINLPs
- Semi-Infinite Programming
- Chance-Constrained Optimization
- Data-Driven Stochastic Optimization
Global Optimization of Two-Stage Stochastic Programs

K. and Barton. Integrating Benders decomposition and Lagrangian relaxation for solving two-stage stochastic MINLPs
K. and Barton. GOSSIP: Decomposition software for the global optimization of two-stage stochastic MINLPs
Subramanian, K., et al. Optimization under uncertainty of a hybrid waste tire & natural gas flexible polygeneration system
Global Optimization of Two-Stage Stochastic Programs

- Complexity of generic B&B grows exponentially with number of scenarios
- Designed first fully-decomposable algorithm with provable convergence

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\[ \nu_\alpha^* := \min_{x \in X} f(x) \]
\[ \text{s.t. } \mathbb{P}\{g(x, \xi) \leq 0\} \geq 1 - \alpha \]

- Previous approaches are either suboptimal, or do not scale
Stochastic Approximation for Chance Constraints

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\[ \text{s.t. } \mathbb{P}\{g(x, \xi) \leq 0\} \geq 1 - \alpha \]

- Previous approaches are either suboptimal, or do not scale
- Designed a stochastic subgradient method for approximating the efficient frontier of cost versus risk (\(\nu^*_\alpha \) vs \( \alpha \))

Better Integration of Renewables in the Power Grid

- Generators balance renewables variability by activating reserves via piecewise-affine policy
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- Generators balance renewables variability by activating reserves via piecewise-affine policy
  - Less conservative than forcing affine policy to be feasible with high probability
- Tailored decomposition method for DC-OPF. Our approach yields solutions with
  - Lower total cost and Higher wind utilization

\[ \begin{array}{c}
\text{Expected total cost (incl. pen.)} \\
\text{Wind penetration [%]} \\
\end{array} \]

\[ \begin{array}{c}
\text{Expected wind utilization [%]} \\
\text{Wind penetration [%]} \\
\end{array} \]

□: our approach. Δ: generator penalty. ○ and ×: chance constraints

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Optimization Under Uncertainty

General optimization model with uncertain parameters $Y$:

$$\min_{z \in \mathcal{Z}} c(z, Y)$$

- $\mathcal{Z}$ is the feasible region (assume known) for decisions $z$
- $Y$ is a vector of uncertain parameters $\Rightarrow$ ill-posed problem
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Popular modeling approaches:

1. **Stochastic**: assuming distribution of $Y$ known, minimize expected/average system cost

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

2. **Robust**: assuming support of $Y$ known, minimize worst-case system cost

   $$\min_{z \in \mathcal{Z}} \max_{y \in Y} c(z, y)$$
Traditional Data-Driven Stochastic Programming

• Traditional SP: minimize expected system cost assuming feasible region $\mathcal{Z}$ and distribution of $Y$ known

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

• Data-driven SP: have access to samples $\{y_i\}_{i=1}^n$ of $Y$

$$\min_{z \in \mathcal{Z}} \mathbb{E}_Y [c(z, Y)] \approx \min_{z \in \mathcal{Z}} \frac{1}{n} \sum_{i=1}^n c(z, y_i) \quad \text{(SAA)}$$

• Sample Average Approximation theory: as sample size $n \to \infty$, optimal value and solutions converge at the rate $O_p \left( n^{-1/2} \right)$

How can we use covariates $X$ to better predict the random vector $Y$?
Traditional Data-Driven Stochastic Programming

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Jim Luedtke  
(UW-Madison ISyE)  

Güzin Bayraksan  
(OSU ISE)  

Nam Ho-Nguyen  
(USYD Business)
Stochastic Programming with Covariate Information

Power Grid Scheduling

\( Y \): Load; Renewable energy outputs  
\( X \): Weather observations; Time/Season  
\( z \): Generator scheduling decisions

Production Planning/Scheduling

\( Y \): Product demands; Prices  
\( X \): Seasonality; Web search results  
\( z \): Production and inventory decisions

Portfolio Optimization

\( Y \): Stock returns  
\( X \): Historical returns; Economic indicators  
\( z \): Investment decisions
Stochastic Programming with Covariate Information

• Assume we have uncertain parameter and covariate data pairs

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

• When making decision \( z \), we observe a new covariate \( X = x \)

• Goal: minimize expected cost given covariate observation \( x \):

\[ \min_{z \in Z} \mathbb{E} [c(z, Y) \mid X = x] \]
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• How to construct data-driven approximation to conditional SP?
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• How to construct data-driven approximation to conditional SP?

1. Learn: predict \( Y \) given \( X = x \)
2. Optimize: integrate learning into optimization (with errors)
Stochastic Programming with Covariate Information

- Assume we have uncertain parameter and covariate data pairs

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- When making decision \( z \), we observe a new covariate \( X = x \)
- **Goal:** minimize expected cost given covariate observation \( x \):

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- **Challenge:** \( \mathcal{D}_n \) may not include covariate observation \( X = x \)
- **How to construct data-driven approximation to conditional SP?**
  1. Learn: predict \( Y \) given \( X = x \)
  2. Optimize: integrate learning into optimization (with errors)

- Assume \( Y = f^*(X) + Q^*(X)\varepsilon \) with \( X \) and \( \varepsilon \) independent
Traditional Integrated Learning and Optimization

1. Use data to train your favorite ML prediction model:

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

2. Given observed covariate \( X = x \), use point prediction within deterministic optimization model

\[ \min_{z \in Z} c(z, \hat{f}_n(x)) \]
Traditional Integrated Learning and Optimization

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- Modular: separate learning and optimization steps
- Expect to work well only if prediction is highly accurate
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- Modular: separate learning and optimization steps
- Expect to work well only if prediction is highly accurate
- Many recently proposed improvements in the literature, e.g., Ban and Rudin (2019); Bertsimas and Kallus (2020); Deng and Sen (2022); Donti et al. (2017); Elmachtoub and Grigas (2022)
Empirical Residuals-based Sample Average Approximation

1. Estimate $f^*$, $Q^*$ using your favorite ML method $\Rightarrow \hat{f}_n, \hat{Q}_n$

K., Ho-Nguyen, and Luedtke. Data-driven multistage stochastic optimization on time series. Working Paper
Empirical Residuals-based Sample Average Approximation

1 Estimate $f^*$, $Q^*$ using your favorite ML method $\Rightarrow \hat{f}_n, \hat{Q}_n$

Compute *empirical residuals* $\hat{e}^i_n := [\hat{Q}_n(x^i)]^{-1}(y^i - \hat{f}_n(x^i))$, $i \in [n]$
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Compute empirical residuals $\hat{\varepsilon}_n^i := [\hat{Q}_n(x^i)]^{-1}(y^i - \hat{f}_n(x^i)), i \in [n]$

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

$$\min_{z \in \mathcal{Z}} \frac{1}{n} \sum_{i=1}^{n} c(z, \hat{f}_n(x) + \hat{Q}_n(x)\hat{\varepsilon}_n^i) \quad \text{(ER-SAA)}$$
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- Modular like traditional approach

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- Modular like traditional approach

**Contributions:**

- General convergence analysis
- Improvements when sample size is small
- Extension to dynamic/sequential decision-making


K., Ho-Nguyen, and Luedtke. Data-driven multistage stochastic optimization on time series. Working Paper
New Small Sample Variant of ER-SAA

Mitigate effects of overfitting by using *leave-one-out residuals*

1. Estimate $f^*$, $Q^*$ separately with each data point $i$ left out (leave-one-out regression) $\Rightarrow \hat{f}_i(\cdot), \hat{Q}_i(\cdot)$ for $i \in [n]$
New Small Sample Variant of ER-SAA

Mitigate effects of overfitting by using \textit{leave-one-out residuals}

1 Estimate $f^*$, $Q^*$ separately with each data point $i$ left out
   (leave-one-out regression) $\Rightarrow \hat{f}_{-i}(\cdot), \hat{Q}_{-i}(\cdot)$ for $i \in [n]$

Compute \textit{leave-one-out residuals} $\hat{\varepsilon}_n^i := [\hat{Q}_{-i}(x^i)]^{-1}(y^i - \hat{f}_{-i}(x^i)), i \in [n]$
New Small Sample Variant of ER-SAA

Mitigate effects of overfitting by using \textit{leave-one-out residuals}

1. Estimate $f^*$, $Q^*$ separately with each data point $i$ left out (leave-one-out regression) $\Rightarrow \hat{f}_{-i}(\cdot), \hat{Q}_{-i}(\cdot)$ for $i \in [n]$

Compute \textit{leave-one-out residuals} $\hat{\varepsilon}_i^n := [\hat{Q}_{-i}(x^i)]^{-1}(y^i - \hat{f}_{-i}(x^i)), i \in [n]$

2. Use $\{\hat{f}_n(x) + \hat{Q}_n(x)\hat{\varepsilon}_i^n\}_{i=1}^n$ or $\{\hat{f}_{-i}(x) + \hat{Q}_{-i}(x)\hat{\varepsilon}_i^n\}_{i=1}^n$ as proxy for samples of $Y$ given $X = x$

$$\min_{z \in \mathcal{Z}} \frac{1}{n} \sum_{i=1}^{n} c(z, \hat{f}_n(x) + \hat{Q}_n(x)\hat{\varepsilon}_i^n) \quad \text{(J-SAA)}$$

Inspired by Jackknife methods (Barber et al., 2021)
Distributionally robust optimization (ER-DRO)

- Minimize worst-case expected cost over a set of distributions

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

\[ \hat{P}_n(x) = \text{“confidence region” for distribution of } Y \text{ given } X = x \]

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- \[ \hat{P}_n(x) := \left\{ \frac{1}{n} \sum_{i=1}^{n} \delta_{\hat{f}_n(x) + \hat{Q}_n(x) \hat{e}_i} \right\} \implies \text{ER-SAA} \]

- Motivation: DRO regularizes small sample ER-SAA, yielding solutions with better out-of-sample performance
Distributionally robust optimization (ER-DRO)

• Minimize worst-case expected cost over a set of distributions

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• Motivation: DRO regularizes small sample ER-SAA, yielding solutions with better out-of-sample performance

• Example: Wasserstein ambiguity sets of order \( p \in [1, +\infty) \):

\[
\hat{P}_n(x) := \left\{ \text{distributions } Q \text{ such that the } p\text{-Wasserstein distance between } Q \text{ and } \hat{P}_n^{ER}(x) \leq \zeta_n(x) \right\}
\]
Toward Convergence Theory: Definitions

Recall

\[ v^*(x) = \min_{z \in \mathcal{Z}} \mathbb{E}_\varepsilon [c(z, f^*(x) + Q^*(x)\varepsilon)] \]

= optimal value of true conditional SP

\[ \hat{z}^{ER}_n(x) = \text{ER-SAA solution} \]

Asymptotic optimality: the out-of-sample cost of data-driven solutions approaches the optimal value of the true conditional SP as the sample size increases

\[ \mathbb{E}_\varepsilon [c(\hat{z}^{ER}_n(x), f^*(x) + Q^*(x)\varepsilon)] \xrightarrow{p} v^*(x) \]
Toward Convergence Theory: Definitions

Recall

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

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Asymptotic optimality: the out-of-sample cost of data-driven solutions approaches the optimal value of the true conditional SP as the sample size increases

\[ \mathbb{E}_\varepsilon [c(\hat{z}^{ER}_n(x), f^*(x) + Q^*(x)\varepsilon)] \overset{P}{\rightarrow} v^*(x) \]

Setting: two-stage stochastic mixed-integer linear programs with continuous recourse and r.h.s. uncertainty

From hereon, assume for simplicity that \( Q^* \equiv I \)
Asymptotic Optimality of ER-SAA Solutions

Assumption: The regression procedure satisfies

• Pointwise error consistency: \( \hat{f}_n(x) \overset{p}{\rightarrow} f^*(x) \) for a.e. \( x \)

• Mean-squared estimation error consistency: 
  \[
  \frac{1}{n} \sum_{i=1}^{n} \| f^*(x_i) - \hat{f}_n(x_i) \|^2 \overset{p}{\rightarrow} 0.
  \]

Informal Theorem (Asymptotic Optimality)
Under the above assumptions \(†\), the ER-SAA solution \( \hat{z}_{ER_n}(x) \) is asymptotically optimal for a.e. \( x \), i.e.,

\[
E_{\varepsilon}[c(\hat{z}_{ER_n}(x), f^*(x) + \varepsilon)] \overset{p}{\rightarrow} v^*(x) \]

\(†\) Plus some mild standard assumptions on the true conditional SP, see arXiv:2207.13554
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\(^\dagger\)Plus some mild standard assumptions on the true conditional SP, see arXiv:2207.13554
Finite-Sample Guarantees for ER-SAA Solutions

Estimate sample size $n$ required for optimal solutions of ER-SAA to be $\kappa$-optimal to the true conditional SP with probability $\geq 1 - \delta$
Finite-Sample Guarantees for ER-SAA Solutions

Estimate sample size $n$ required for optimal solutions of ER-SAA to be $\kappa$-optimal to the true conditional SP with probability $\geq 1 - \delta$

- If $f^*$ is linear and we use OLS regression, then require

  $$n \geq O(\kappa^2 \log(\kappa) + d_x d_y \log(\kappa))$$

- If $f^*$ is $s$-sparse linear and we use the Lasso, then require

  $$n \geq O(\kappa^2 \log(\kappa) + sd x \log(\kappa))$$

- If $f^*$ is Lipschitz and we use kNN regression, then require

  $$n \geq O(d_x \kappa^2 \log(\kappa) + (d_x d_y \kappa^2) \log(\kappa))$$
Finite-Sample Guarantees for ER-SAA Solutions

Estimate sample size $n$ required for optimal solutions of ER-SAA to be $\kappa$-optimal to the true conditional SP with probability $\geq 1 - \delta$

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

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

- If $f^*$ is Lipschitz and we use kNN regression, then require
  \[
  n \geq \frac{O(1)d_z}{\kappa^2} \log \left( \frac{O(1)}{\kappa} \right) + \left( \frac{O(1)d_y}{\kappa^2} \right)^{d_x} \left[ d_x \log \left( \frac{O(1)d_x d_y}{\kappa^2} \right) + \log \left( \frac{O(1)}{\delta} \right) \right]
  \]
Choosing the Ambiguity Set Radius for Wasserstein 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

\[
P\{\|f^*(x) - \hat{f}_n(x)\|_p > \kappa_{p,n}(\alpha, x)\} \leq \alpha,
\]

and

\[
P\left\{\frac{1}{n} \sum_{i=1}^{n} \|f^*(x_i) - \hat{f}_n(x_i)\|_p > \kappa_{p,n}(\alpha, x)\right\} \leq \alpha.
\]

Example: Finite-sample guarantee on regression step holds for OLS, Lasso with

\( \kappa_{2,2}(\alpha, x) = O(n^{-1} \log(\alpha^{-1})) \)

CART, RF with

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$$

and

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

and

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

Example: Finite-sample guarantee on regression step holds for $p = 2$ and

- OLS, Lasso with $\kappa_{2,n}^2(\alpha, x) = O(n^{-1} \log(\alpha^{-1}))$
- CART, RF with $\kappa_{2,n}^2(\alpha, x) = O(n^{-1} \log(\alpha^{-1}))^{O(1)/d_x}$
Choosing the Ambiguity Set Radius for Wasserstein 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

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

\[
\mathbb{P}\left\{ \frac{1}{n} \sum_{i=1}^{n} \| f^*(x^i) - \hat{f}_n(x^i) \|^p > \kappa_{p,n}(\alpha, x) \right\} \leq \alpha.
\]

Given covariate realization \( x \) and risk level \( \alpha \in (0, 1) \), use radius

\[
\zeta_n(\alpha, x) := 2\kappa_{p,n}\left(\frac{\alpha}{4}, x\right) + \overline{k}_{p,n}\left(\frac{\alpha}{2}\right)
\]

\( \overline{k}_{p,n}\left(\frac{\alpha}{2}\right) \) := traditional Wasserstein radius used if we know \( f^* \) (Kuhn et al., 2019)

**Guarantees**

\[
\mathbb{P}\{ d_W(\hat{P}_n^{ER}(x), P_{Y|X=x}) > \zeta_n(\alpha, x) \} \leq \alpha
\]
Informal Theorem (Finite Sample Certificate)

For the above choice of the Wasserstein radius $\zeta_n(\alpha, x)$, the solution $\hat{z}^{DRO}_n(x)$ and the optimal value $\hat{v}^{DRO}_n(x)$ satisfy

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

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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 the sequence $\{\hat{z}^{DRO}_n(x)\}$ of solutions satisfies

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

- Meet demands of 30 customer types for 20 resources (two-stage stochastic LP with r.h.s. uncertainty)

- Uncertain demands $Y$ generated according to

$$Y_j = \alpha_j^* + \sum_{l=1}^{3} \beta_{jl}^*(X_l)^\theta + \varepsilon_j, \quad \forall j \in \{1, \cdots, 30\},$$

where $\varepsilon_j \sim \mathcal{N}(0, \sigma_j^2)$, $\theta \in \{0.5, 1, 2\}$, $\text{dim}(X) \in \{10, 100\}$
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- Fit linear model with OLS/Lasso regression (even when $\theta \neq 1$)

$$Y_j = \alpha_j + \sum_{l=1}^{\text{dim}(X)} \beta_{jl} X_l + \eta_j, \quad \forall j \in \{1, \cdots, 30\},$$

where $\eta_j$ are zero-mean errors

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

Green (k): ER-SAA+kNN

Blue (O): ER-SAA+OLS

Black (R): Reweighted SAA with kNN (Bertsimas and Kallus, 2020)
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Lower y-axis value $\implies$ closer to optimal

![Box plots showing the performance of different models with varying dimensions and sample sizes.](image)
Results with Correct Model Class ($\theta = 1$)

Green (k): ER-SAA+kNN

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

Boxes: 25, 50, and 75 percentiles of 99% upper confidence bounds

Whiskers: 5 and 95 percentiles

Sample sizes: $\{5, 20, 100\} \times (\text{dim}(X) + 1)$
Results with Misspecified Model Class ($\theta \neq 1$)

O: ER-SAA+OLS, k: ER-SAA+kNN, R: Reweighted SAA with kNN

$\theta = 0.5$

$\theta = 2$
Advantage of J-SAA, Modularity with Limited Data \((\theta = 1)\)

Black (J): J-SAA+OLS,  Green (O): ER-SAA+OLS,  Blue (L): ER-SAA+Lasso

Lower y-axis value \(\Rightarrow\) closer to optimal

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Part 1: 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
- Ongoing: multistage stochastic opt. for time series data
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Future work

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

1. Research Overview
2. Stochastic Programming with Covariate Information
3. Learning to Accelerate the Global Optimization of QCQPs
Motivation

Many important applications can be formulated as nonconvex QCQPs

AC Optimal Power Flow

The Pooling Problem

Inputs | Pools | Outputs
Motivation

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Often, wish to *repeatedly* solve instances of the same nonconvex problem with different data, e.g., loads, wind, qualities, prices
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AC Optimal Power Flow

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Can we exploit *shared structure* to accelerate global solution?

Harsha Nagarajan
(LANL)

Deepjyoti Deka
(LANL)
Global Optimization of QCQPs

Consider the following class of QCQPs:

\[
\nu^* := \min_{x,w} c^T x + d^T w
\]

s.t. \( w_{ij} = x_i x_j, \quad \forall (i,j) \in B, \)

\[ A x + B w \leq b, \quad x \in [-1, 1]^{d_x} \]

- The bilinear constraints are what make the problem hard
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- The bilinear constraints are what make the problem hard
- Get feasible solutions/upper bounds using local optimization
- Obtain lower bounds on \( \nu^* \) using relaxations
Relaxing Bilinear Terms

The feasible region of the **hard bilinear** constraints
\[ w_{ij} = x_i x_j, \quad x_i, x_j \in [-1, 1] \]  \hspace{1cm} (1)

is a subset of the feasible region of the **easy linear** constraints
\[
\begin{align*}
-x_i - x_j - 1 &\leq w_{ij} \leq x_i - x_j + 1, \\
-x_i - x_j - 1 &\leq w_{ij} \leq x_i - x_j + 1,
\end{align*}
\]  \hspace{1cm} (2)

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Relaxing Bilinear Terms

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\[
- x_i - x_j - 1 \leq w_{ij} \leq x_i - x_j + 1, \\
- x_i + x_j - 1 \leq w_{ij} \leq x_j - x_i + 1,
\]

\[ x_i, x_j \in [-1, 1] \quad (2) \]

Replace bilinear constraints (1) in the QCQP with McCormick Relaxations (2) to determine a valid lower bound

\[ \nu^* \geq \nu^M := \min_{x, w} c^T x + d^T w \]

s.t. \( Ax + Bw \leq b, \)

\[- x_i - x_j - 1 \leq w_{ij} \leq x_i - x_j + 1, \quad \forall (i, j) \in B, \]

\[- x_i + x_j - 1 \leq w_{ij} \leq x_j - x_i + 1, \quad \forall (i, j) \in B, \]

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-\quad x_i + x_j - 1 \leq w_{ij} \leq x_j - x_i + 1, \quad \forall (i, j) \in B, \\
-\quad x \in [-1, 1]^{d_x}
\]

Typically $\nu^M \ll \nu^*$, and the gap is closed using continuous B&B
Tighten Relaxations By Partitioning Variable Domains

- Partition variable domains into “disjoint” subintervals, e.g.,
  \[ x_1 \in [-1, 0] \text{ OR } [0, 1] \]
  \[ x_2 \in [-1, 0] \text{ OR } [0, 1] \]
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- Construct Piecewise McCormick Relaxations on the variable partitions and solve a MIP to obtain lower bound

\[ \nu^* \geq \nu^{PMR} := \min_{x, w} c^T x + d^T w \]

s.t. \( Ax + Bw \leq b, \)

\[ (x_i, x_j, w_{ij}) \in PMR_{ij}(p_i, p_j), \quad \forall (i, j) \in B, \]

\[ x \in [-1, 1]^{d_x}, \]

where \( p_i \) is the vector of partitioning points for \( x_i \)
The Lower Part of the Piecewise McCormick Relaxations

Partitions: $x_1 \in [-1, 0] \text{ OR } [0, 1], \quad x_2 \in [-1, 0] \text{ OR } [0, 1]$
Refine Variable Partitions for Convergence

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\text{s.t. } \begin{align*}
Ax + Bw &\leq b, \\
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• Refine variable partitions to close gap between \( \nu^{PMR} \) and \( \nu^* \)
  e.g. \[ x_1 \in [-1, -0.5] \text{ OR } [-0.5, 0] \text{ OR } [0, 1] \]
  \[ x_2 \in [-1, 0] \text{ OR } [0, 0.2] \text{ OR } [0.2, 1] \]
How to Pick Partitioning Points?

Adaptive strategy in the solver Alpine (Nagarajan et al., 2019): refine partitions around a reference point \( \bar{x} \) (e.g., around a feasible point or solution to McCormick relaxation)
How to Pick Partitioning Points?

Adaptive strategy in the solver Alpine (Nagarajan et al., 2019): refine partitions around a reference point $\bar{x}$ (e.g., around a feasible point or solution to McCormick relaxation)

- Example: if $\bar{x} = (0.3, 0)$ and parameter $\Delta = 4$

  $\begin{align*}
  -0.2 & \quad \bar{x}_1 & \quad 0.8 \\
  -1 & \quad 0.3 & \quad 1 \\
  \end{align*}$

  width $= \frac{1 - (-1)}{\Delta}$

  $\begin{align*}
  -0.5 & \quad \bar{x}_2 & \quad 0.5 \\
  -1 & \quad 0 & \quad 1 \\
  \end{align*}$

Can we choose better partitioning points for faster convergence?

More partitioning points $\Rightarrow$ tighter lower bounds at the expense of harder MIPs
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\[
\begin{align*}
\Delta & = 4 & 10 & 15 \\
\text{Time for Ex1:} & 5087s & \textbf{704s} & 1551s \\
\text{Time for Ex2:} & \textbf{2632s} & 5023s & 6642s \\
\text{Time for Ex3:} & 3000s & 4540s & \textbf{1433s}
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\end{align*}
$$

width = $\frac{1 - (-1)}{\Delta}$

Best choice of $\Delta$ can vary depending on instance
(illustration on 3 random QCQPs)

<table>
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<tr>
<th>$\Delta$</th>
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Can we choose better partitioning points for faster convergence?
More partitioning points $\implies$ tighter lower bounds at the expense of harder MIPs
Strong Partitioning (SP) to Improve Choice of Partitions

New Approach: Choose partitioning points to maximize the lower bound

\[ p^* \in \arg \max_{p \in P} \nu^{PMR}(p), \]

- \( p_i \) is the vector of partitioning points for \( x_i \)

\[ \nu^{PMR}(p) := \min_{x, w} c^T x + d^T w \]

s.t. \( Ax + Bw \leq b, \)

\[ (x_i, x_j, w_{ij}) \in PMR_{ij}(p_i, p_j), \quad \forall (i, j) \in B, \]

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- From iteration 2, use aforementioned partitioning strategy (guaranteed to converge irrespective of points chosen by SP)
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How to solve this max-min problem (locally)?
Using generalized gradients of value function \(\nu^{PMR}\) within a bundle solver
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**How to solve this max-min problem (locally)?**

Using generalized gradients of value function \( \nu^{PMR} \) within a bundle solver

**Solving this max-min problem may be as hard as solving the QCQP!**
Using ML to Accelerate Partitioning (Within Alpine)

Given family of random QCQPs of the form (Bao et al., 2009)

\[ \nu^*(\theta) := \min_{x,w} c(\theta)^T x + d(\theta)^T w \]

s.t. \( A(\theta)x + B(\theta)w \leq b, \)
\[ w_{ij} = x_i x_j, \quad \forall (i,j) \in B, \]
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Parameters \( \theta \) vary from one instance to the next

Test instances
\( d_x \in \{10, 20, 50\} \)
5\( d_x \) bilinear terms
\( d_x \) bilinear inequalities
\( d_x/5 \) linear equalities
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**Input:** underlying problem, distribution of parameters \( \theta \)

**Output:** ML model that predicts partitioning points given \( \bar{\theta} \)

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- Solve max-min problem to determine “optimal” partitioning points for each training instance

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- Learn an ML model \( \theta^i \mapsto \text{optimal partitioning points} \)
  (use scikit-learn’s AdaBoostRegressor with 10-fold CV)
- Use ML model to predict partitioning points for new instance \( \bar{\theta} \)
Numerical Results for Random QCQPs
Results for $d_x = 20$ variables

- Generate 1000 random QCQPs with varying parameters $\theta$
- determine 2/4 SP points per variable for each instance
- Eliminate partitioning points that aren’t useful
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![Graph showing numerical results for random QCQPs with $d_x = 20$ variables.](image)
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<td>16.0</td>
</tr>
<tr>
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</tr>
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<td>29.9</td>
<td>6.0</td>
</tr>
<tr>
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<td>10.0</td>
<td>0.9</td>
</tr>
<tr>
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<td>3.3</td>
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</tr>
<tr>
<td>&lt; 0.5x</td>
<td>0.2</td>
<td>3.3</td>
</tr>
</tbody>
</table>

Average Speedup (Shifted GM):
Alpine+SP: 5.1x, Alpine+ML: 2.1x
Alpine+SP4: 9x, Alpine+ML4: 2.3x
Numerical Results for Random QCQPs

Results for $d_x = 20$ variables

- Generate 1000 random QCQPs with varying parameters $\theta$
- determine 2/4 SP points per variable for each instance
- Eliminate partitioning points that aren’t useful

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Average Speedup (Shifted GM):
- Alpine+SP: 5.1x, Alpine+ML: 2.1x
- Alpine+SP4: 9x, Alpine+ML4: 2.3x
Numerical Results for the Pooling Problem

- 45 sources, 15 pools, 30 terminals, 1 quality
  (124/572 variables part. in 261 bilinear terms)
- 1000 random instances with $\theta =$ input qualities
- 2 SP points per variable (total $124 \times 2$)
Numerical Results for the Pooling Problem

- 45 sources, 15 pools, 30 terminals, 1 quality (124/572 variables part. in 261 bilinear terms)
- 1000 random instances with $\theta =$ input qualities
- 2 SP points per variable (total $124 \times 2$)
- Feature dimension: 667, Output dimension: 248
Numerical Results for the Pooling Problem

- 45 sources, 15 pools, 30 terminals, 1 quality (124/572 variables part. in 261 bilinear terms)
- 1000 random instances with $\theta =$ input qualities
- 2 SP points per variable (total $124 \times 2$)
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Average Speedup (Shifted GM):
Alpine+SP: 3.6x, Alpine+ML: 2.1x
Part 2: Concluding Remarks

Strong Partitioning provides an excellent benchmark for ML to accelerate partitioning algorithms for global optimization

- SP reduces Alpine’s solution time by $4x - 16x$ on average (max. speedups of $15x - 700x$)
- SP can reduce Alpine’s first iteration gap by more than $2000x$!
- Off-the-shelf ML model improves Alpine’s run time by $2x - 4.5x$ on average (max. speedups of $10x - 200x$)
Part 2: Concluding Remarks

Strong Partitioning provides an excellent benchmark for ML to accelerate partitioning algorithms for global optimization

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- SP can reduce Alpine’s first iteration gap by more than 2000x!
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Ongoing and future work

- Techniques for adaptive strong partitioning
- Investigate tailored ML models to imitate SP
- Extend SP to broader optimization classes, including MINLPs
- Explore application to AC optimal power flow


ER-SAA
Numerical Study: Optimal Resource Allocation

\[
\min_{z \geq 0} c^T z + \mathbb{E}_Y [Q(z, Y)]
\]

- \(z_i\): quantity of resource \(i \in \mathcal{I}\) (order before demands realized)
- \(Y_j\): uncertain demand of customer type \(j \in \mathcal{J}\)

\[
Q(z, Y) := \min_{w, v \geq 0} d^T w
\]

\[
\text{s.t. } \sum_{j \in \mathcal{J}} v_{ij} \leq z_i, \quad \forall i \in \mathcal{I},
\]

\[
\sum_{i \in \mathcal{I}} \mu_{ij} v_{ij} + w_j \geq Y_j, \quad \forall j \in \mathcal{J}.
\]

- \(v_{ij}\): amount of resource \(i\) allocated to customer type \(j\)
- \(w_j\): amount of customer type \(j\) demand that is not met
- \(\mu_{ij} \geq 0\): service rate of resource \(i\) for customer type \(j\)
Wasserstein ER-DRO
Choosing the Radius for Wasserstein ER-DRO 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 $\mathcal{D}_n$ to choose $\zeta_n$ independently of the covariate realization $X = x$
  ▶ Approach 3: Use both the data $\mathcal{D}_n$ and the covariate realization $X = x$ to choose the radius $\zeta_n(x)$

• Approach 3 is more data intensive than Approaches 1 & 2
Numerical Study: Mean-CVaR 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-CVaR 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 $\bar{\varepsilon}_j \sim N(0, 0.025j)$, $\omega \sim N(0, 0.02)$, $\theta \in \{0.5, 1, 2\}$, $\dim(X) \in \{10, 100\}$

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

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

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 ($\theta = 1$)

**E:** ER-SAA + OLS

1, 2 & 3: Wasserstein radius specified using Approaches 1, 2 & 3

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

Boxes: 25, 50, and 75 percentiles of 99% upper confidence bounds

Whiskers: 5 and 95 percentiles

Sample sizes: $\{5, 10, 20, 50\} \times (\text{dim}(X) + 1)$
Results with OLS and Misspecified Model Class ($\theta \neq 1$)

$\theta = 0.5$

$\theta = 2$

$\mathbf{d}_x = 10$

$\mathbf{d}_x = 100$
Data-Driven Multistage Stochastic Optimization on Time Series
Numerical Study: Hydrothermal Scheduling

\[
\min \sum_{t} \text{generation \& spillage costs at time } t
\]

s.t. at each time stage \( t \):

- reservoir volume increase = rainfall - generation
- thermal + hydro generation = demand
- bounds on reservoir height, generation amounts

- **Uncertain rainfall** at each time stage \( t \)
Multistage Stochastic Optimization

Complexity of multi-stage stochastic programs can grow significantly with the number of stages $T$!
Multistage Stochastic Optimization

Consider the multistage stochastic program

\[
V_t(x_{t-1}, \xi[t]) := \min_{x_t \in X_t(x_{t-1}, \xi_t)} f_t(x_t, \xi_t) + \mathbb{E} \left[ V_{t+1}(x_t, \xi_{t+1}) \mid \xi[t] \right], \quad t \in [T - 1],
\]

\[
V_T(x_{T-1}, \xi[T]) := \min_{x_T \in X_T(x_{T-1}, \xi_T)} f_T(x_T, \xi_T) \quad \text{(MSSP)}
\]

- **Decision Process:** \( \xi_1 \leadsto x_1 \leadsto \xi_2 \leadsto x_2 \leadsto \cdots \xi_T \leadsto x_T \)
- **Time Series:** \( \xi[t] := (\xi_1, \xi_2, \ldots, \xi_t) \), where \( \{\xi_t\} \) is a stochastic process satisfying

\[
\xi_t = m_t^*(\xi_{t-1}, \epsilon_t), \quad \forall t \in \mathbb{Z}
\]

We deal with multi-stage stochastic LPs, where

- \( f_t(x_t, \xi_t) := c_t^\top x_t \)
- \( X_t(x_{t-1}, \xi_t) := \{x_t \in \mathbb{R}^{nt}_+ : B_t(\xi_t)x_{t-1} + A_t x_t = h_t(\xi_t)\} \)
Problem Setup

• Given historical data from a single trajectory of \( \{\xi_t\} \)

\[
\mathcal{D}_n := \left\{ \tilde{\xi}_s, \tilde{\xi}_{s+1}, \ldots, \tilde{\xi}_{s+n} \right\}
\]

• Want to solve

\[
V_1(x_0, \xi_1) := \min_{x_1 \in \mathcal{X}_1(x_0, \xi_1)} f_1(x_1, \xi_1) + \mathbb{E} \left[ V_2(x_1, \xi_2) \mid \xi_1 \right],
\]

where

\[
V_t(x_{t-1}, \xi_t) := \min_{x_t \in \mathcal{X}_t(x_{t-1}, \xi_t)} f_t(x_t, \xi_t) + \mathbb{E} \left[ V_{t+1}(x_t, \xi_{t+1}) \mid \xi_t \right], \quad t \in \left[ T - 1 \right],
\]

\[
V_T(x_{T-1}, \xi_T) := \min_{x_T \in \mathcal{X}_T(x_{T-1}, \xi_T)} f_T(x_T, \xi_T).
\]

• Assume
  
  • True model: \( \xi_t = f^*(\xi_{t-1}) + Q^*(\xi_{t-1})\varepsilon_t \) with i.i.d. errors \( \{\varepsilon_t\} \)
  
  • We know function classes \( \mathcal{F}, \mathcal{Q} \) such that \( f^* \in \mathcal{F}, Q^* \in \mathcal{Q} \)
Empirical Residuals-based Sample Average Approximation

Extension of the two-stage approach

1. Estimate $f^*$, $Q^*$ using our favorite ML method $\Rightarrow \hat{f}_n$, $\hat{Q}_n$

Compute empirical residuals

$$\hat{\epsilon}_n^i := [\hat{Q}_n(\tilde{\xi}_{s+i-1})]^{-1}(\tilde{\xi}_{s+i} - \hat{f}_n(\tilde{\xi}_{s+i-1})), \quad i \in [n]$$

2. Use $\{\hat{f}_n(\xi_t) + \hat{Q}_n(\xi_t)\hat{\epsilon}_n^i\}_{i=1}^n$ as proxy for samples of $\xi_{t+1}$ given $\xi_t$

$$\hat{V}_{t,n}^{ER}(x_{t-1}, \xi_t) := \min_{x_t \in X_t(x_{t-1}, \xi_t)} f_t(x_t, \xi_t) + \frac{1}{n} \sum_{j \in [n]} \hat{V}_{t+1,n}^{ER}(x_t, \hat{f}_n(\xi_t) + \hat{Q}_n(\xi_t)\hat{\epsilon}_n^i)$$

- Modular like traditional approach
- Only require a single trajectory of $\{\xi_t\}$
- Tailored convergence analysis required since same empirical errors used in each time stage
Numerical Experiments: Hydrothermal Scheduling

- **Decisions** $z_t$: Hydrothermal & natural gas generation, spillage
- **Random vector** $\xi$: Amount of rainfall
Numerical Experiments: Hydrothermal Scheduling

Assume true time series model for rainfall is of the form

\[ \xi_t = (\alpha_t^* + \beta_t^* \xi_{t-1}) \exp(\varepsilon_t), \]

where \[ \alpha_t^* = \alpha_{t+12}^*, \quad \beta_t^* = \beta_{t+12}^*, \quad \varepsilon_t \text{ i.i.d. } \sim \mathcal{N}(\mu, \Sigma) \]

Good fit to historical data over 8 decades!
Numerical Experiments: Hydrothermal Scheduling

- Consider the Brazilian interconnected power system with four hydrothermal reservoirs

- Generate a sample trajectory of $\{\xi_t\}$ using time series model

$$
\xi_t = (\alpha_t^* + \beta_t^* \xi_{t-1}) \exp(\varepsilon_t),
$$

where $\alpha_t^* = \alpha_{t+12}^*$, $\beta_t^* = \beta_{t+12}^*$, $\varepsilon_t \sim i.i.d. \mathcal{N}(\mu, \Sigma)$

- Estimate coefficients $(\hat{\alpha}_t, \hat{\beta}_t)$ such that

$$
\hat{\alpha}_t = \hat{\alpha}_{t+12}, \quad \hat{\beta}_t = \hat{\beta}_{t+12}
$$

Use these to estimate samples of the errors $\varepsilon_t$

- Solve the ER-SAA model using SDDP.jl

Estimate sub-optimality of ER-SAA solutions
Results when the time series model is correctly specified

Estimate true heteroscedastic model:  
\[ \xi_t = (\alpha_t^* + \beta_t^* \xi_{t-1}) \exp(\varepsilon_t) \]

Lower y-axis value \(\implies\) closer to optimal

\(n\): number of historical samples per month

Boxes: 25, 50, and 75 percentiles of optimality gap estimates; Whiskers: 5 and 95 percentiles
Results when the time series model is misspecified

Estimate seasonal additive error model: \[ \xi_t = \alpha_t^* + \beta_t^* \xi_{t-1} + \epsilon_t \]

Lower y-axis value \(\implies\) closer to optimal

\(n\): number of historical samples per month

Boxes: 25, 50, and 75 percentiles of optimality gap estimates; Whiskers: 5 and 95 percentiles
Using ML to Accelerate Global Optimization
Using ML to Accelerate Partitioning Algorithms

Input: underlying problem, distribution of parameters $\theta$

Output: ML model that predicts partitioning points given $\bar{\theta}$

• Generate **1000** training samples $\{\theta^i\}$ of problem parameters $\theta$
• Solve max-min problem to determine “optimal” partitioning points for each training instance
• Learn an ML model $\theta^i \mapsto$ optimal partitioning points
• Use ML model to predict partitioning points for new instance $\bar{\theta}$

Use Scikit-learn’s AdaBoostRegressor to train Regression Trees with max_depth = 25, num_estimators = 1000 (no tuning!)

• Features for training and prediction:
  ▶ Parameter $\theta$
  ▶ Best found feasible solution during presolve (one local solve)
  ▶ McCormick lower bounding solution (no partitioning)

• Use 10-fold cross validation to generate predictions for $\{\theta^i\}$
Numerical Results for Random QCQPs
Results for $d_x = 10$ variables

- Generate 1000 random QCQPs with varying parameters $\theta$
- For each instance, determine 2 optimal partitioning points per variable by solving a max-min problem
- Eliminate optimal partitioning points that aren’t useful

![Graph showing % instances solved within time T for $d_x = 10$]

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Average Speedup (Shifted GM):
Alpine+SP: 4.5x, Alpine+ML: 3.5x
Numerical Results for Random QCQPs

Results for $d_x = 50$ variables

- Generate 1000 random QCQPs with varying parameters $\theta$
- 2 partitioning points per variable for each instance
- Eliminate partitioning points that aren’t useful

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Average Speedup (Shifted GM):
Alpine+SP: 8.1x, Alpine+ML: 4.2x