Learning-Assisted Data-Driven Optimization

Rohit Kannan

Center for Nonlinear Studies, Applied Mathematics & Plasma Physics
Los Alamos National Laboratory

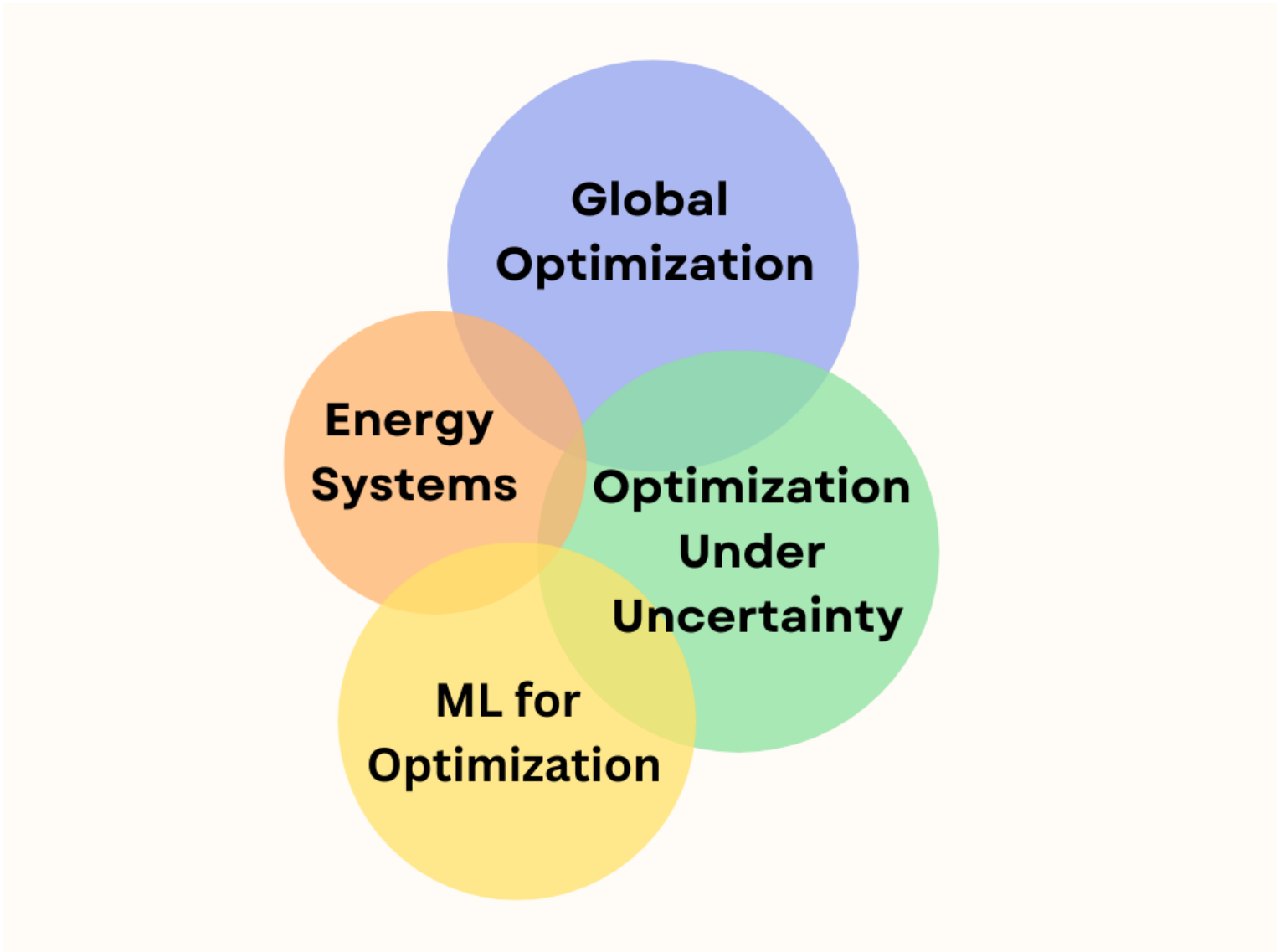
Grado Dept. of Industrial & Systems Engineering, Virginia Tech

February 6, 2023

Funding: U.S. DOE, Center for Nonlinear Studies, LANL LDRD Program

Outline

Research Overview



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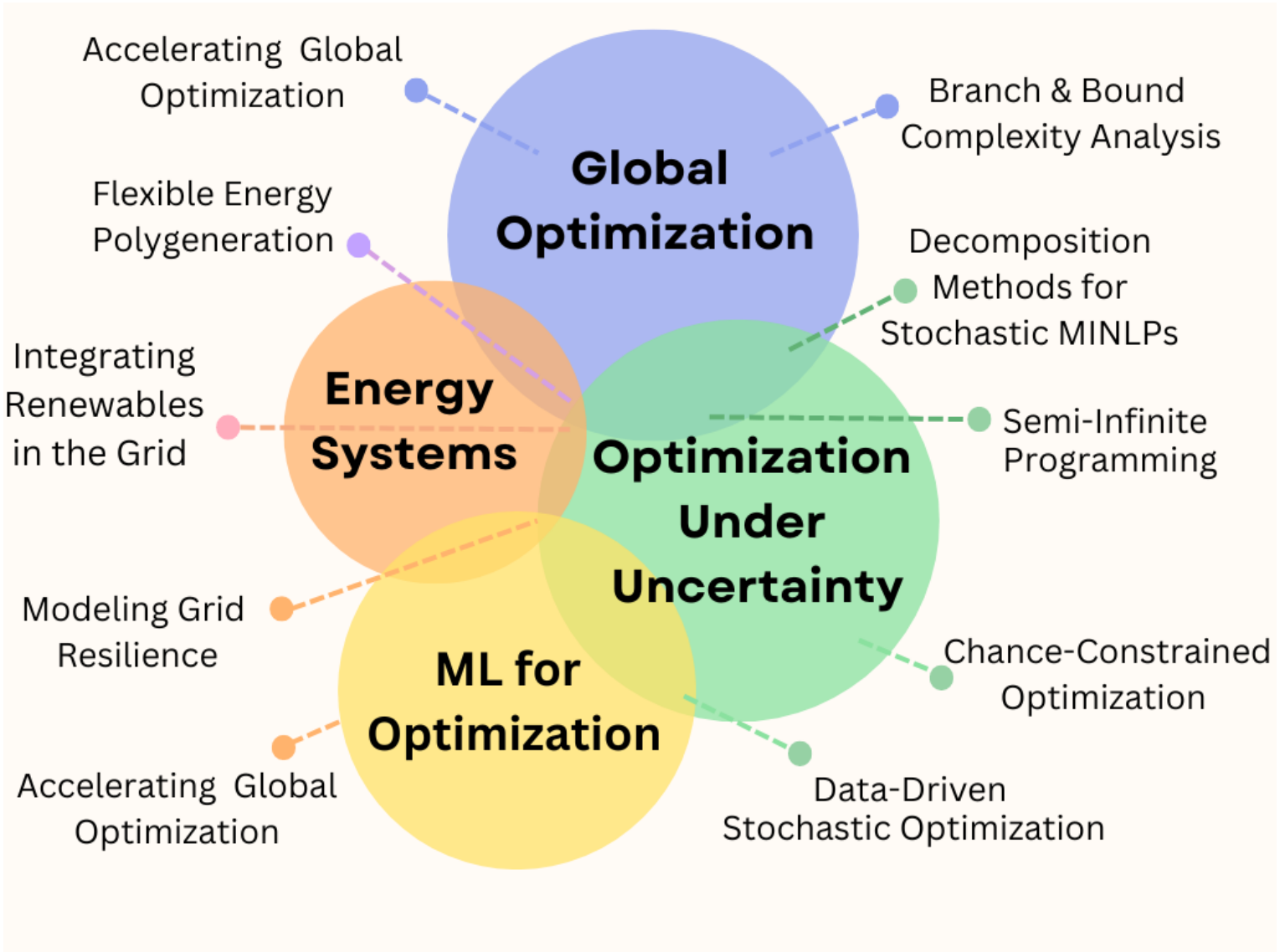
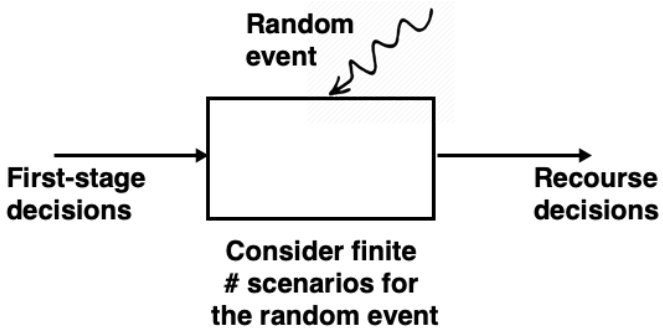
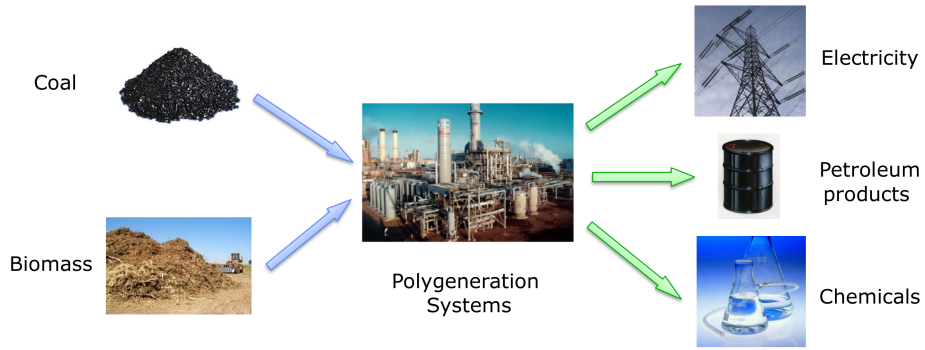


Global Optimization of Two-Stage Stochastic Programs





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

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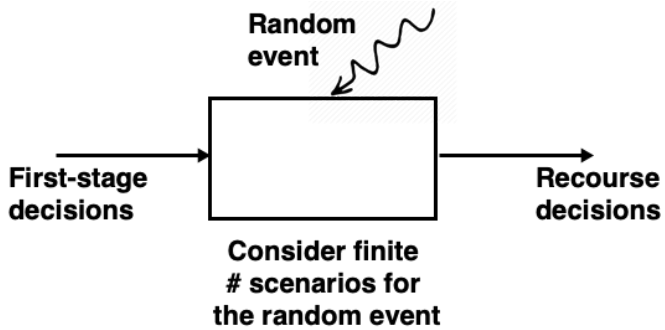

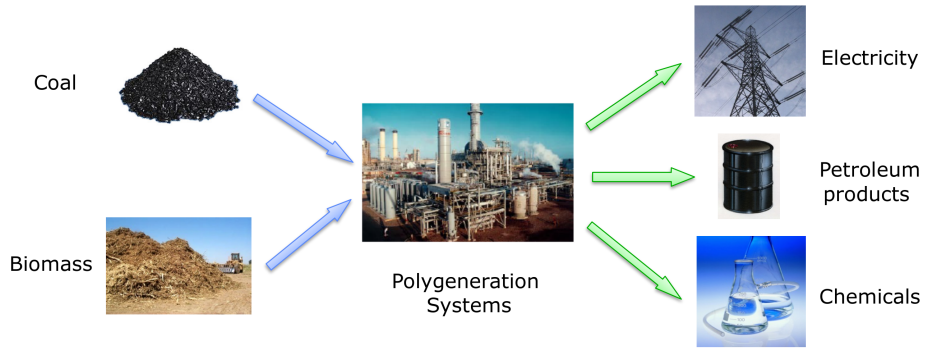

- Complexity of generic B&B grows exponentially with number of scenarios
- Designed first fully-decomposable algorithm with provable convergence

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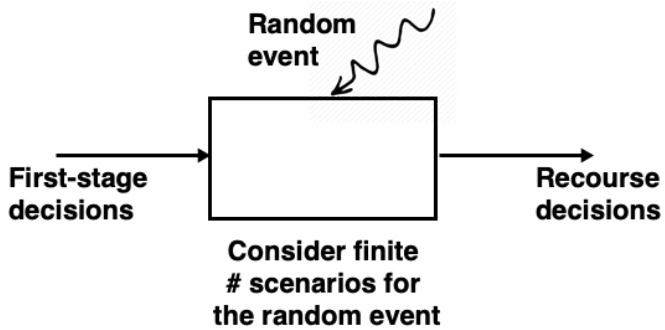

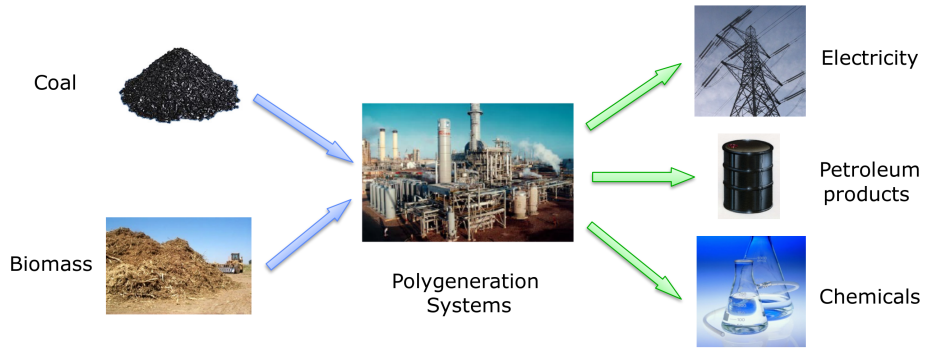

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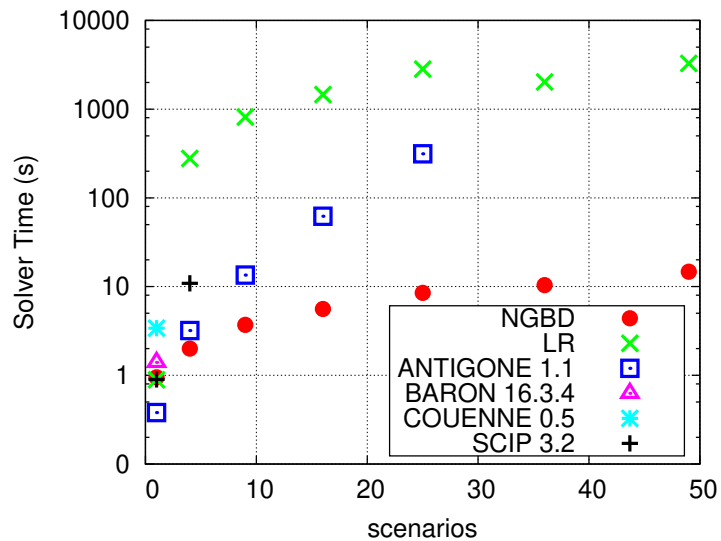

NGBD & LR: decomposition methods
Rest: State-of-the-art solvers

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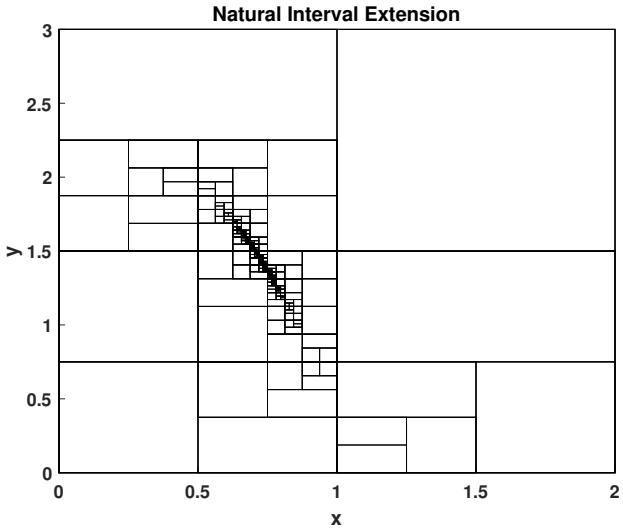
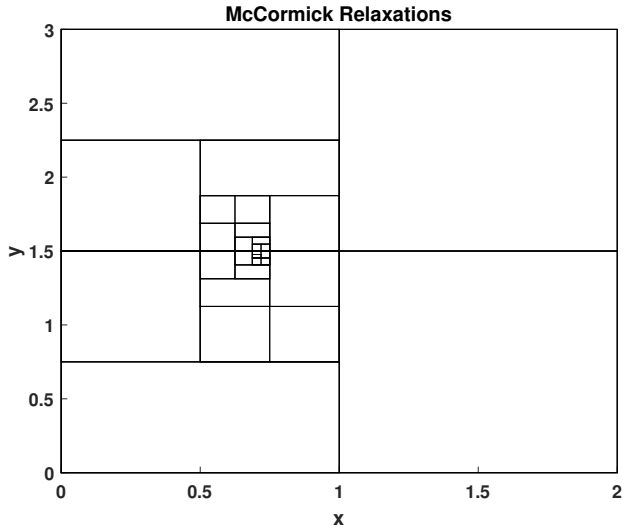
Analysis of the Complexity of B&B Algorithms





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- Built theory to understand which bounding methods can avoid this
  - Important implications for design of reduced-space B&B algorithms

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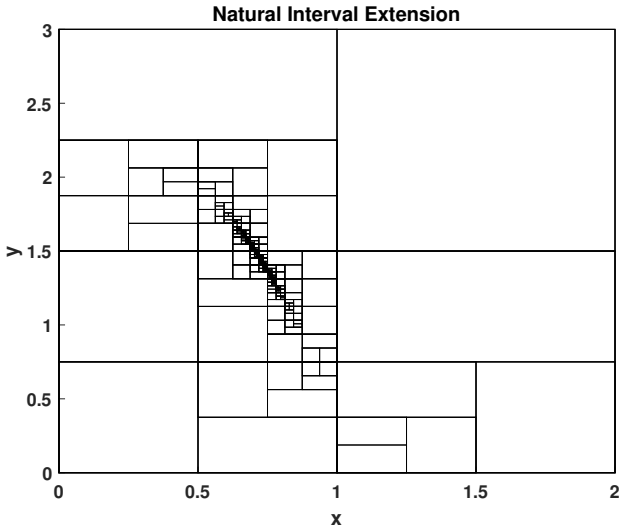

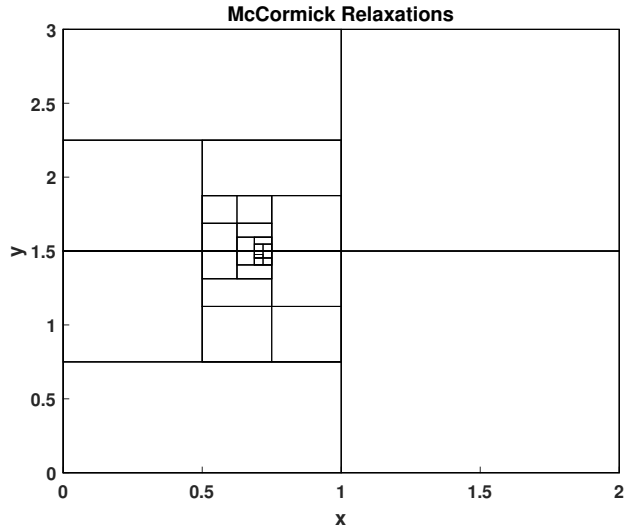

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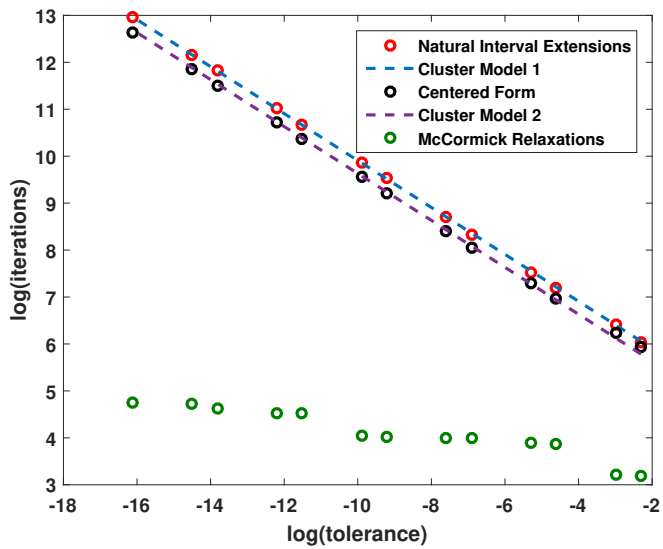

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Stochastic Approximation for Chance Constraints

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

Jim Luedtke
(UW-Madison ISyE)

- Previous approaches are either suboptimal, or do not scale

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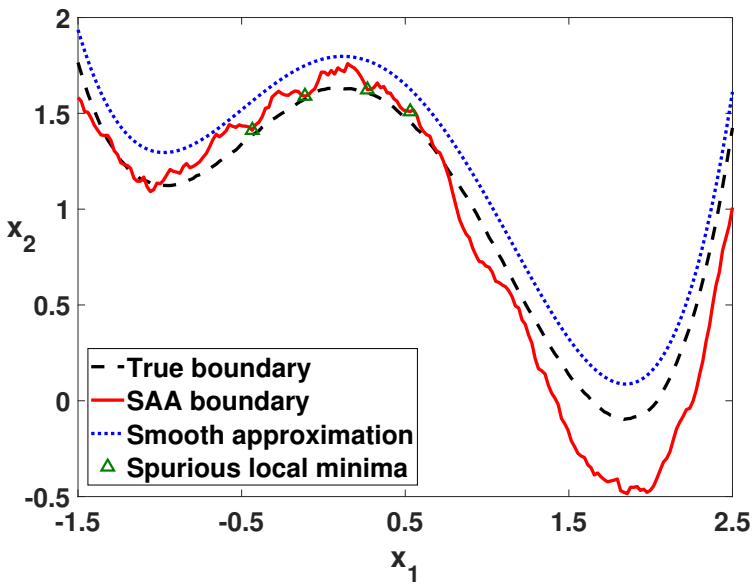
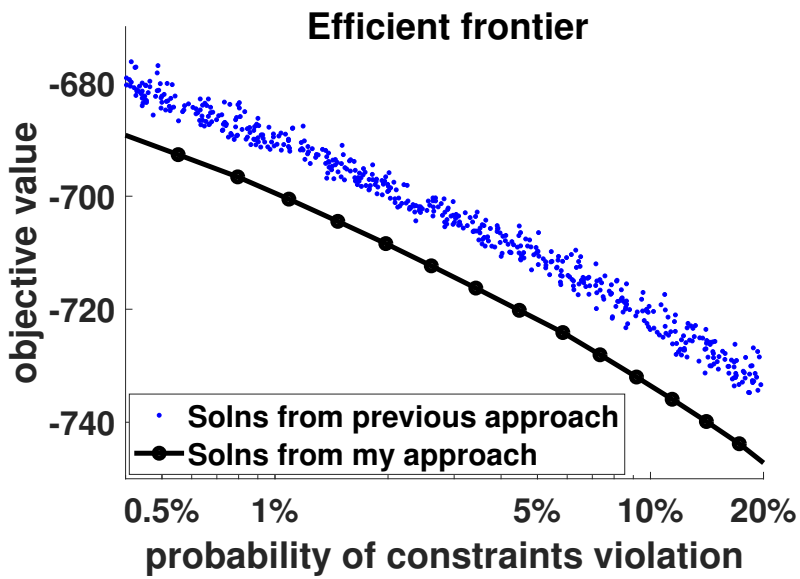
- Previous approaches are either suboptimal, or do not scale
- Designed a stochastic subgradient method for approximating the efficient frontier of cost versus risk (ν_α^* vs α)

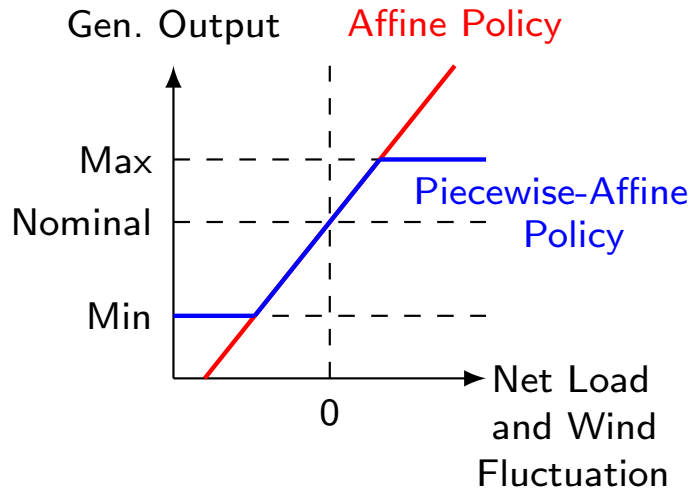




K. and Luedtke (2021). A stochastic approximation method for chance-constrained NLPs. Math. Prog. Comput.

Better Integration of Renewables in the Power Grid

- Generators balance renewables variability by activating reserves via piecewise-affine policy
  - Less conservative than forcing affine policy to be feasible with high probability



Line Roald
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K., Luedtke, and Roald (2020). Stochastic DC-OPF with reserve saturation. Electric Power Systems Research

Better Integration of Renewables in the Power Grid

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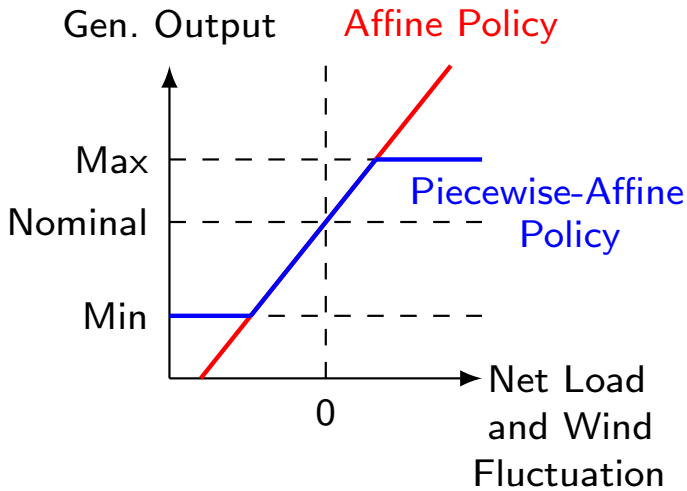
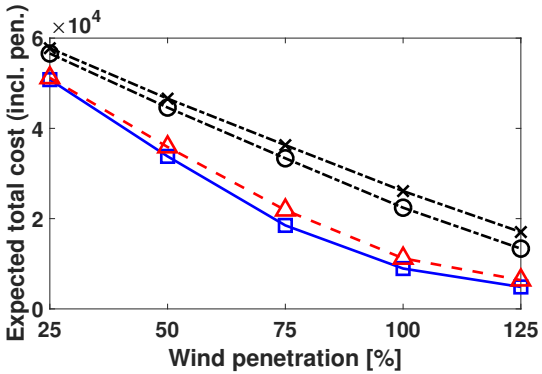
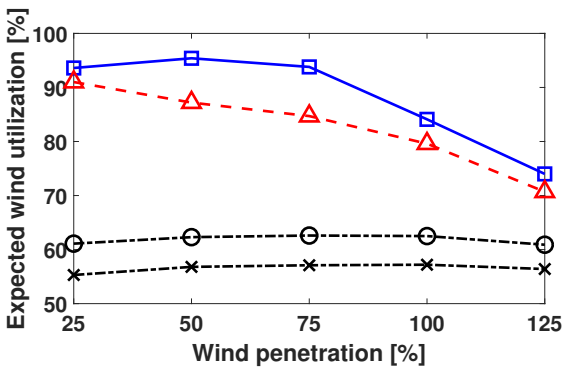
  - Less conservative than forcing affine policy to be feasible with high probability
- Tailored decomposition method for DC-OPF. Our approach yields solutions with



Lower total cost and Higher wind utilization





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□: our approach. △: generator penalty. o and ×: chance constraints

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Outline

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

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

Traditional Data-Driven Stochastic Programming

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

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

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

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

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

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How can we use covariates X to better predict the random vector Y?

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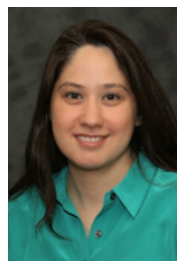
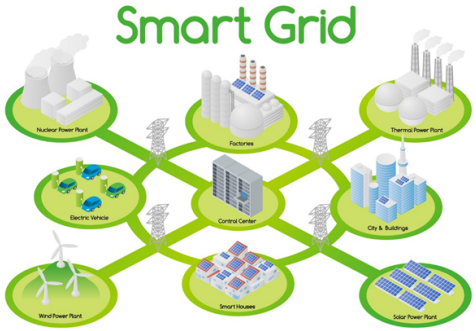


Güzin Bayraksan
(OSU ISE)

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

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

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

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

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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)
- Assume $Y = f^*(X) + Q^*(X)\varepsilon$ with X and ε *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

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- Modular: separate learning and optimization steps
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- 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., Bayraksan, and Luedtke. Data-driven SAA with covariate information. arXiv:2207.13554. Under Revision

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

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

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Contributions:

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

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New Small Sample Variant of ER-SAA

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

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

K., Bayraksan, and Luedtke. Data-driven SAA with covariate information. arXiv:2207.13554. Under Revision

New Small Sample Variant of ER-SAA

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

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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 $X = x$

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

Inspired by Jackknife methods (Barber et al., 2021)

K., Bayraksan, and Luedtke. Data-driven SAA with covariate information. arXiv:2207.13554. Under Revision

Distributionally robust optimization (ER-DRO)

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

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

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

K., Bayraksan, and Luedtke. Residuals-based DRO with covariate information. arXiv:2012.01088. Under Review

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

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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 $p \in [1, +\infty)$:

$$\hat{\mathcal{P}}_n(x) := \{\text{distributions } Q \text{ such that the } p\text{-Wasserstein distance between } Q \text{ and } \hat{P}_n^{ER}(x) \leq \zeta_n(x)\}$$

K., Bayraksan, and Luedtke. Residuals-based DRO with covariate information. arXiv:2012.01088. Under Review

Toward Convergence Theory: Definitions

Recall

- $v^*(x) = \min_{z \in \mathcal{Z}} \mathbb{E}_\varepsilon[c(z, f^*(x) + Q^*(x)\varepsilon)]$
  $= \text{optimal value of true conditional SP}$
- $\hat{z}_n^{ER}(x) = \text{ER-SAA solution}$

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

$$\mathbb{E}_\varepsilon\left[c(\hat{z}_n^{ER}(x), f^*(x) + Q^*(x)\varepsilon)\right] \xrightarrow{p} v^*(x)$$

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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

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Assumption: The regression procedure satisfies

- Pointwise error consistency: $\hat{f}_n(x) \xrightarrow{p} f^*(x)$ for a.e. x
- Mean-squared estimation error consistency:

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

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Informal Theorem (Asymptotic Optimality)

Under the above assumptions†, the ER-SAA solution $\hat{z}_n^{ER}(x)$ is asymptotically optimal for a.e. x, i.e.,

$$\mathbb{E}_\varepsilon\left[c(\hat{z}_n^{ER}(x), f^*(x) + \varepsilon)\right] \xrightarrow{p} v^*(x)$$

†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 κ-optimal to the true conditional SP with probability $\geq 1 - \delta$

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

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

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

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

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

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

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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

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

- OLS, Lasso with $\kappa^2_{2,n}(\alpha, x) = O(n^{-1}\log(\alpha^{-1}))$
- CART, RF with $\kappa^2_{2,n}(\alpha, x) = O(n^{-1}\log(\alpha^{-1}))^{O(1)/d_x}$

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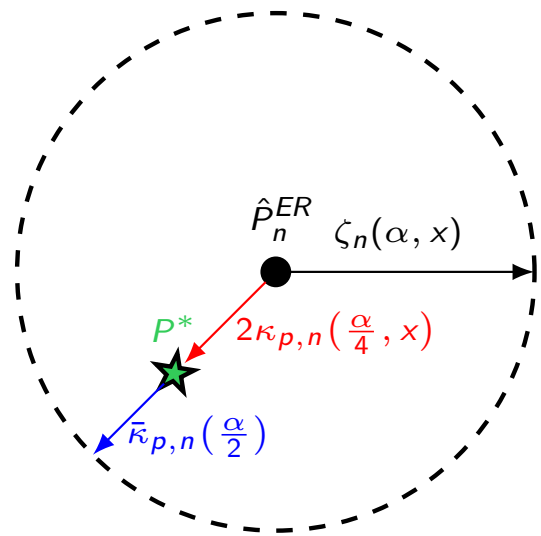
Given covariate realization x and risk level $\alpha \in (0,1)$, use radius

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

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



Guarantees $\mathbb{P}\{d_W(\hat{P}_n^{ER}(x), P_{Y|X=x}) > \zeta_n(\alpha, x)\} \leq \alpha$

Flavor of Wasserstein ER-DRO Results

Informal Theorem (Finite Sample Certificate)

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

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

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

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

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 $\varepsilon_j \sim \mathcal{N}(0, \sigma_j^2)$, $\theta \in \{0.5, 1, 2\}$, $\dim(X) \in \{10, 100\}$

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

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

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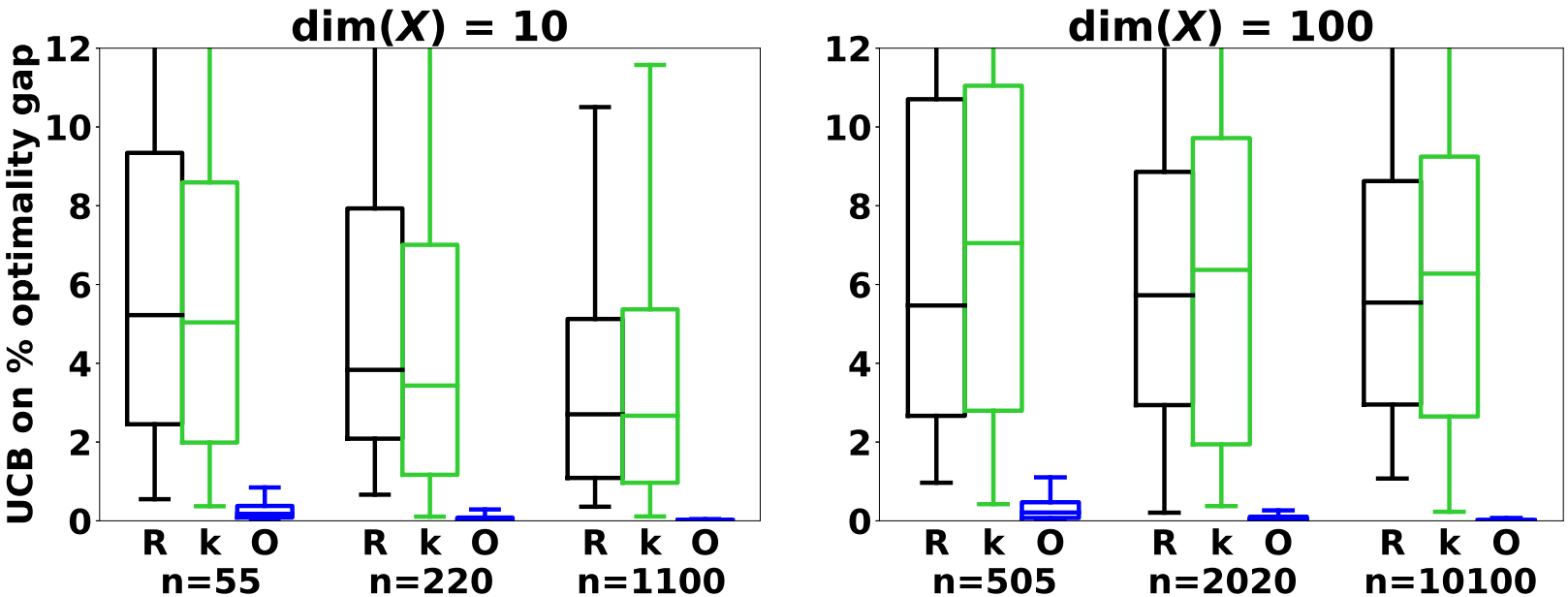
Lower y-axis value $\implies$ closer to optimal



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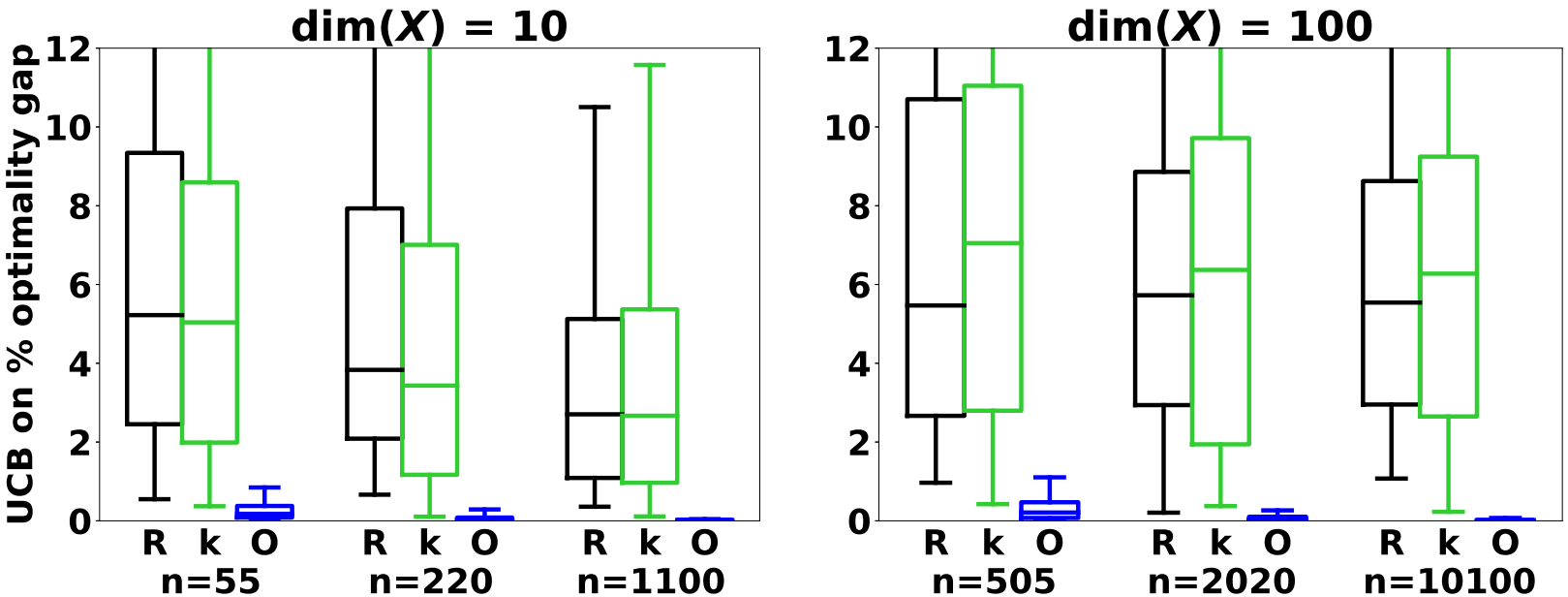


Boxes: 25, 50, and 75 percentiles of 99% upper confidence bounds

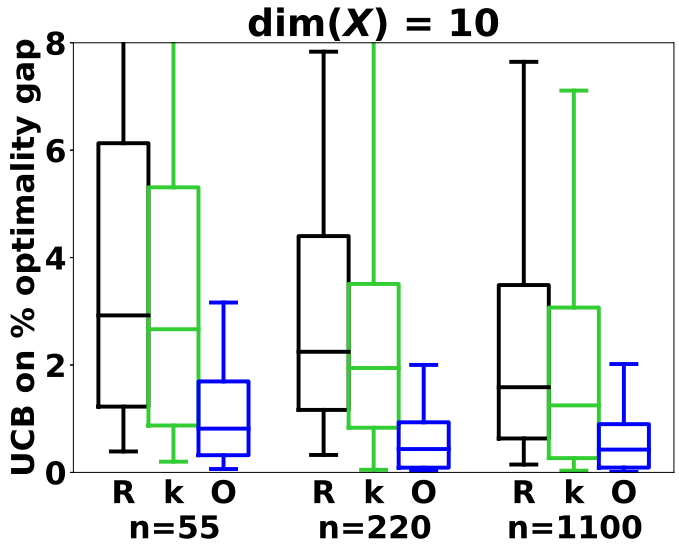
Whiskers: 5 and 95 percentiles

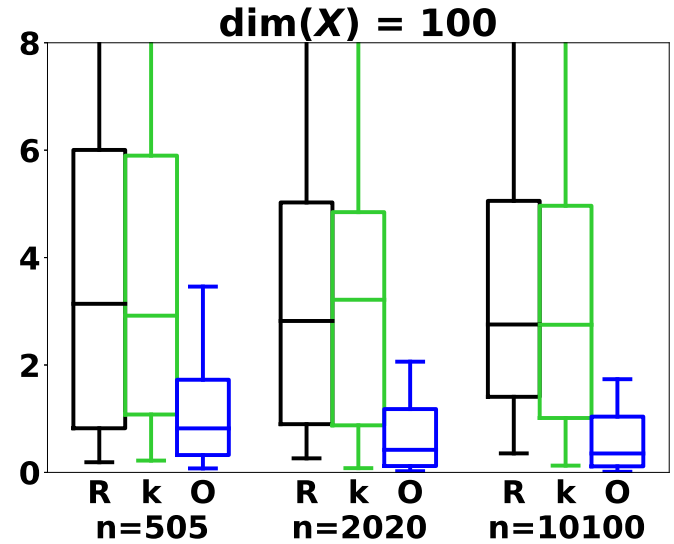
Sample sizes: $\{5, 20, 100\} \times (\dim(X) + 1)$

Results with Misspecified Model Class ($\theta \neq 1$)

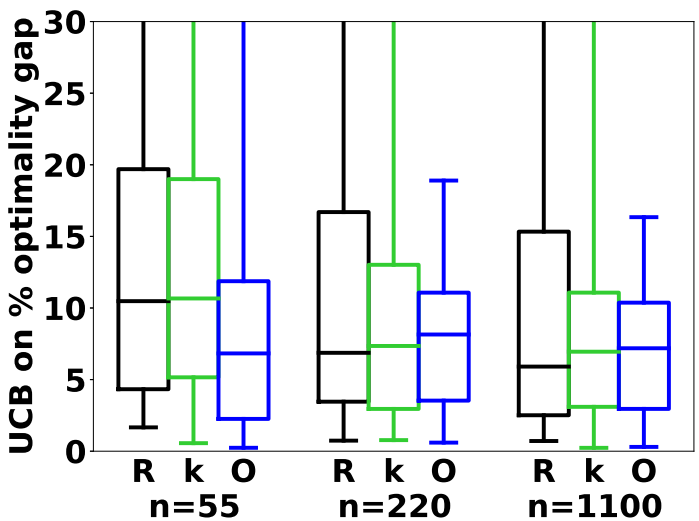
O: ER-SAA+OLS, k: ER-SAA+kNN, R: Reweighted SAA with kNN

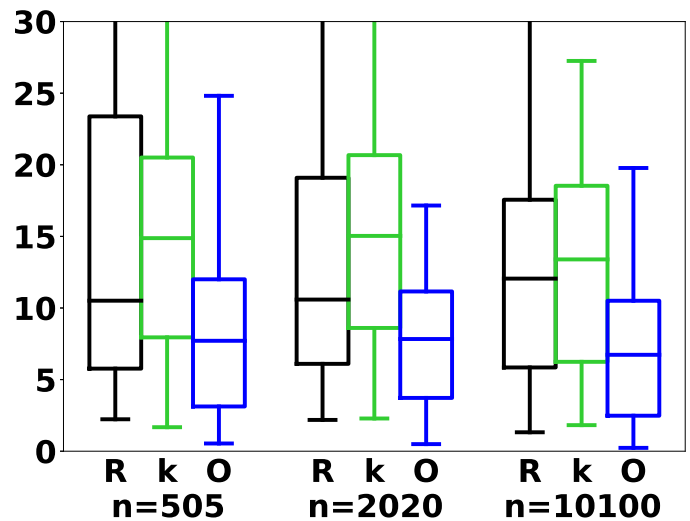
$\theta = 0.5$





$\theta = 2$

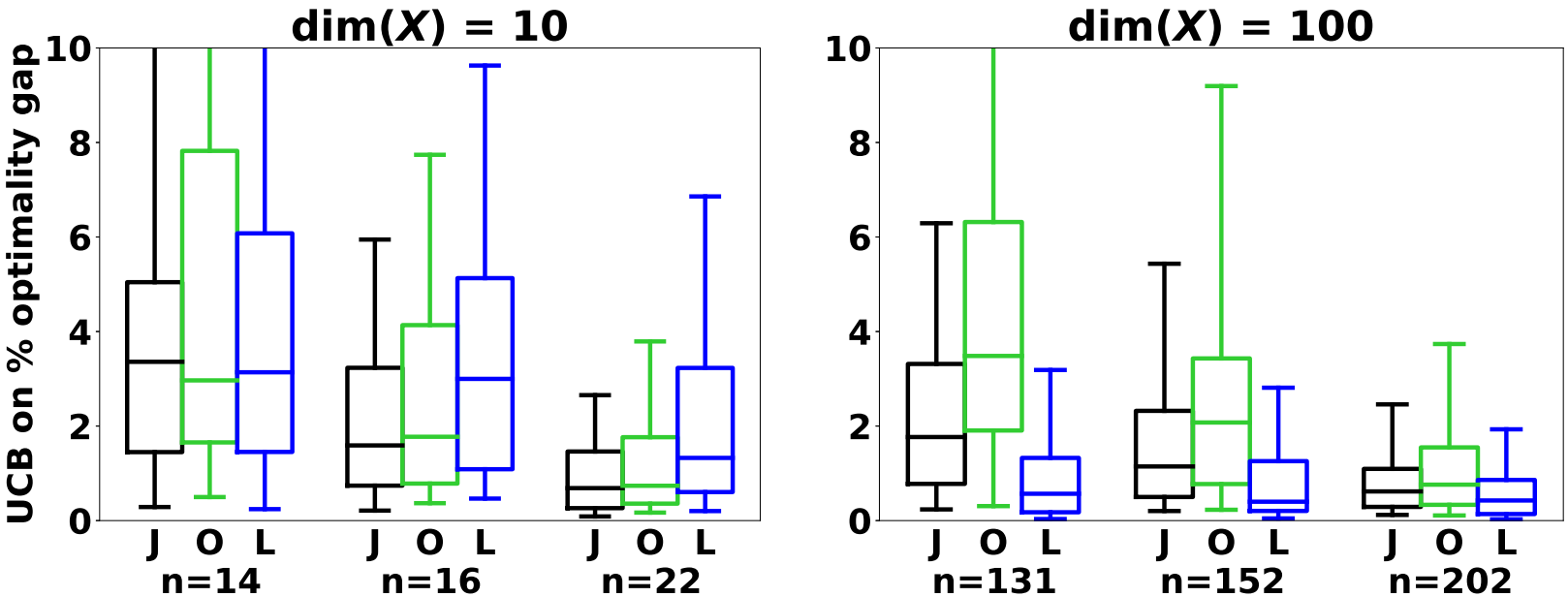




Advantage of J-SAA, Modularity with Limited Data ($\theta = 1$)

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

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



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

Whiskers: 5 and 95 percentiles

Sample sizes: $\{1.3, 1.5, 2\} \times (\dim(X) + 1)$

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
- Preprints: arXiv:2207.13554 and arXiv:2012.01088 with lots of additional theory and experiments
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Future work

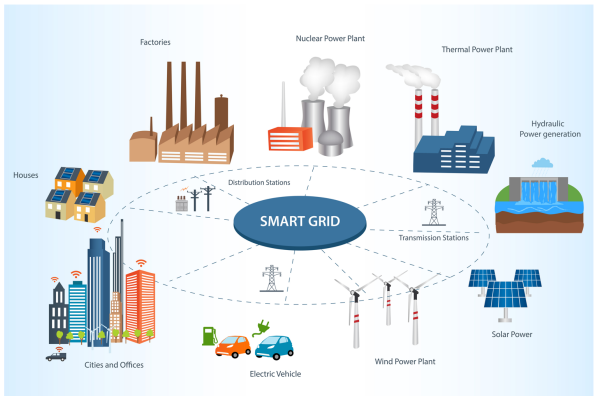
- Formulations with stochastic constraints, discrete recourse decisions; robust multistage optimization
- Application to energy systems optimization

Outline

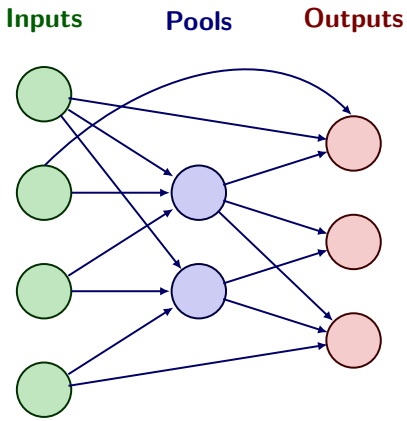
Motivation

Many important applications can be formulated as nonconvex QCQPs

AC Optimal Power Flow



The Pooling Problem



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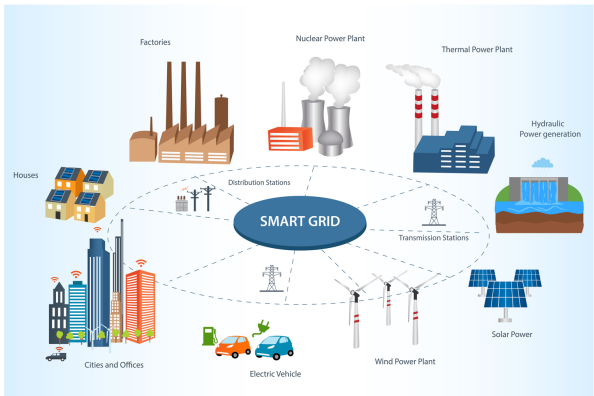

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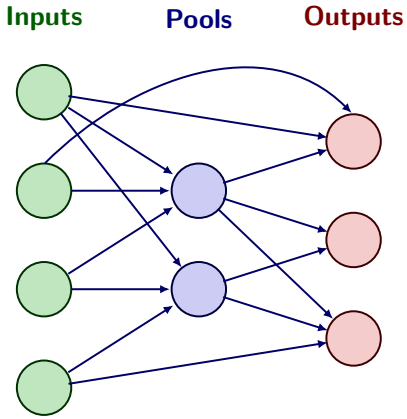

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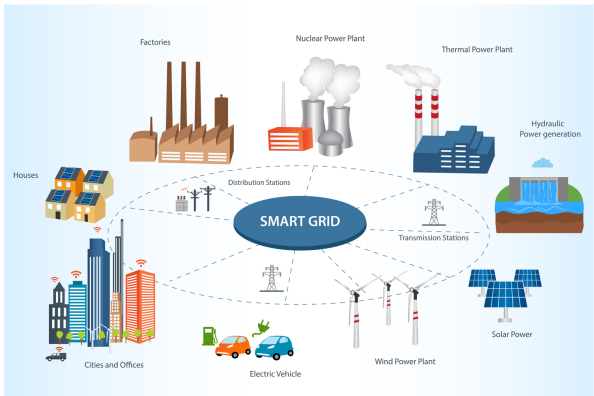

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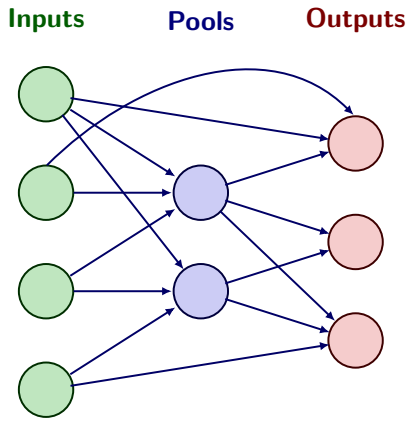

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Can we exploit *shared structure* to accelerate global solution?

Harsha Nagarajan
(LANL)

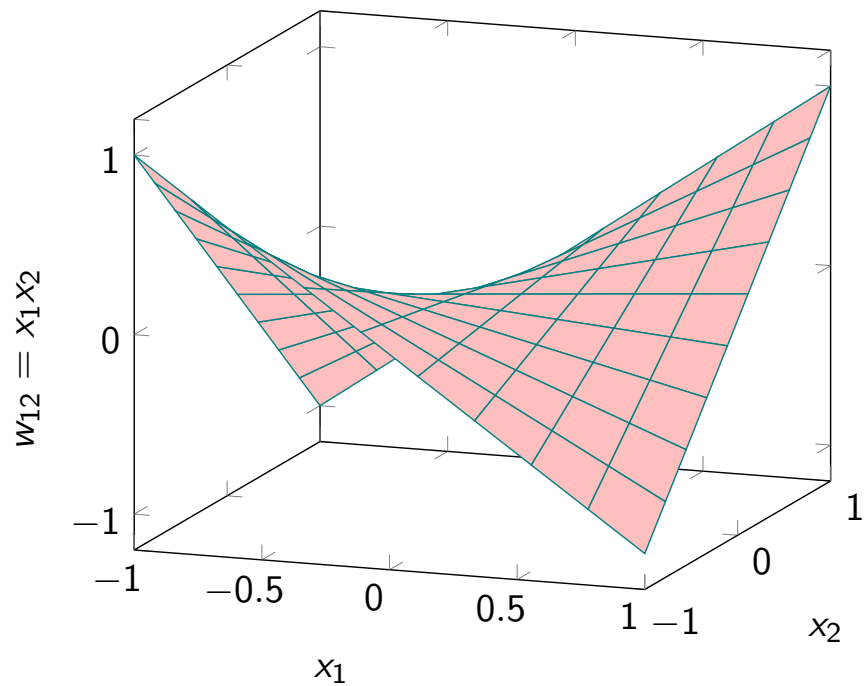
Deepjyoti Deka
(LANL)

Global Optimization of QCQPs

Consider the following class of QCQPs:

$$\begin{aligned} \nu^* := \min_{x,w} \; & c^\mathsf{T} x + d^\mathsf{T} w \\ \text{s.t.} \; & w_{ij} = x_i x_j, \quad \forall (i,j) \in \mathcal{B}, \\ & Ax + Bw \leq b, \;\; x \in [-1,1]^{d_x} \end{aligned}$$

- The bilinear constraints are what make the problem hard



K., Nagarajan, and Deka. Learning to Accelerate the Global Optimization of QCQPs. arXiv:2301.00306. Under Review

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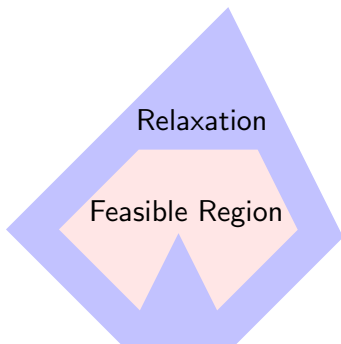
- The bilinear constraints are what make the problem hard
- Get feasible solutions/upper bounds using local optimization
- Obtain lower bounds on ν^* using relaxations



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Relaxing Bilinear Terms

The feasible region of the hard *bilinear* constraints

$$w_{ij} = x_i x_j, \quad x_i, x_j \in [-1, 1] \tag{1}$$

is a subset of the feasible region of the easy *linear* constraints

$$\begin{aligned} -x_i - x_j - 1 \leq w_{ij} \leq x_i - x_j + 1, \\ x_i + x_j - 1 \leq w_{ij} \leq x_j - x_i + 1, \\ x_i, x_j \in [-1, 1] \end{aligned} \tag{2}$$

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

$$\begin{aligned} \nu^* \geq \nu^M := \min_{x,w} \ & c^\mathsf{T} x + d^\mathsf{T} w \\ \text{s.t.} \ & Ax + Bw \leq b, \\ & -x_i - x_j - 1 \leq w_{ij} \leq x_i - x_j + 1, \quad \forall (i,j) \in \mathcal{B}, \\ & x_i + x_j - 1 \leq w_{ij} \leq x_j - x_i + 1, \quad \forall (i,j) \in \mathcal{B}, \\ & x \in [-1, 1]^{d_x} \end{aligned}$$

Relaxing Bilinear Terms

The feasible region of the hard *bilinear* constraints

$$w_{ij} = x_i x_j, \quad x_i, x_j \in [-1, 1] \tag{1}$$

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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.,

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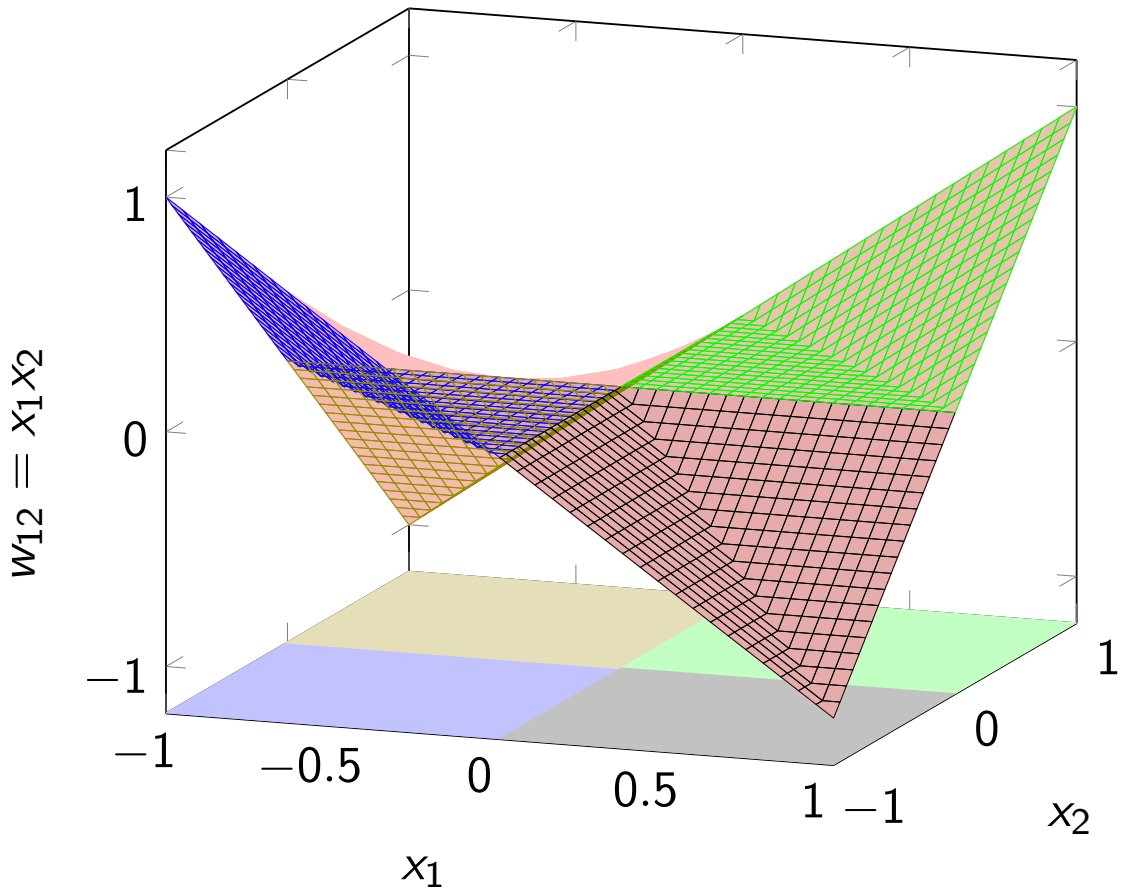
The Lower Part of the Piecewise McCormick Relaxations

Partitions: $x_1 \in [-1, 0]$ OR $[0, 1]$, $\quad x_2 \in [-1, 0]$ OR $[0, 1]$



Refine Variable Partitions for Convergence

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- Refine variable partitions to close gap between ν^{PMR} and ν^*

$$\begin{aligned} \text{e.g.} \quad & x_1 \in [-1, -0.5] \text{ OR } [-0.5, 0] \text{ OR } [0, 1] \\ & x_2 \in [-1, 0] \quad \text{OR } [0, 0.2] \quad \text{OR } [0.2, 1] \end{aligned}$$

How to Pick Partitioning Points?

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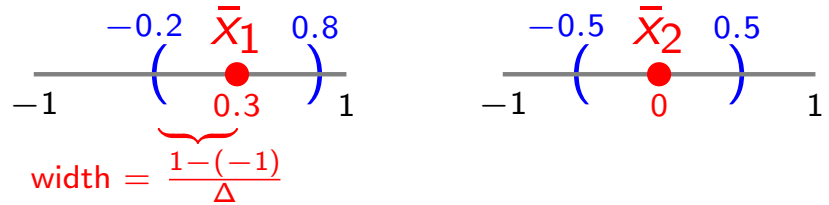

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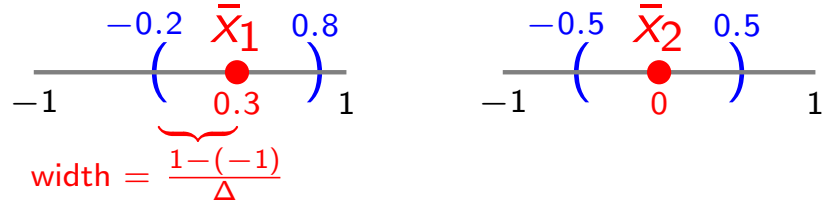

Best choice of Δ can vary depending on instance (illustration on 3 random QCQPs)

Δ	**4**	**10**	**15**
Time for Ex1:	5087s	**704s**	1551s
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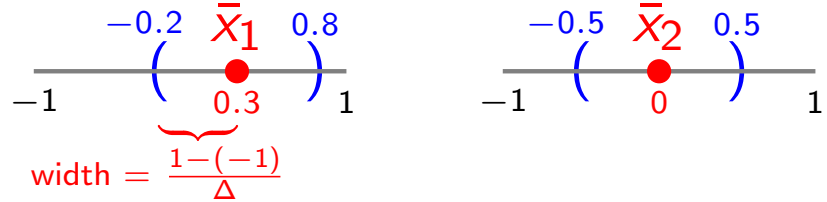

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Can we choose better partitioning points for faster convergence?

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

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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)

$$\begin{aligned} \nu^*(\theta) := \min_{x,w} \; & c(\theta)^\mathsf{T} x + d(\theta)^\mathsf{T} w \\ \text{s.t.} \; & A(\theta)x + B(\theta)w \leq b, \\ & w_{ij} = x_i x_j, \quad \forall (i,j) \in \mathcal{B}, \\ & x \in [0,1]^{d_x} \end{aligned}$$

Test instances

- $d_x \in \{10, 20, 50\}$
- $5d_x$ bilinear terms
- d_x bilinear inequalities
- $d_x/5$ linear equalities

Parameters θ vary from one instance to the next

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- Learn an ML model $\theta^i \mapsto$ `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 θ
- determine 2/4 SP points per variable for each instance
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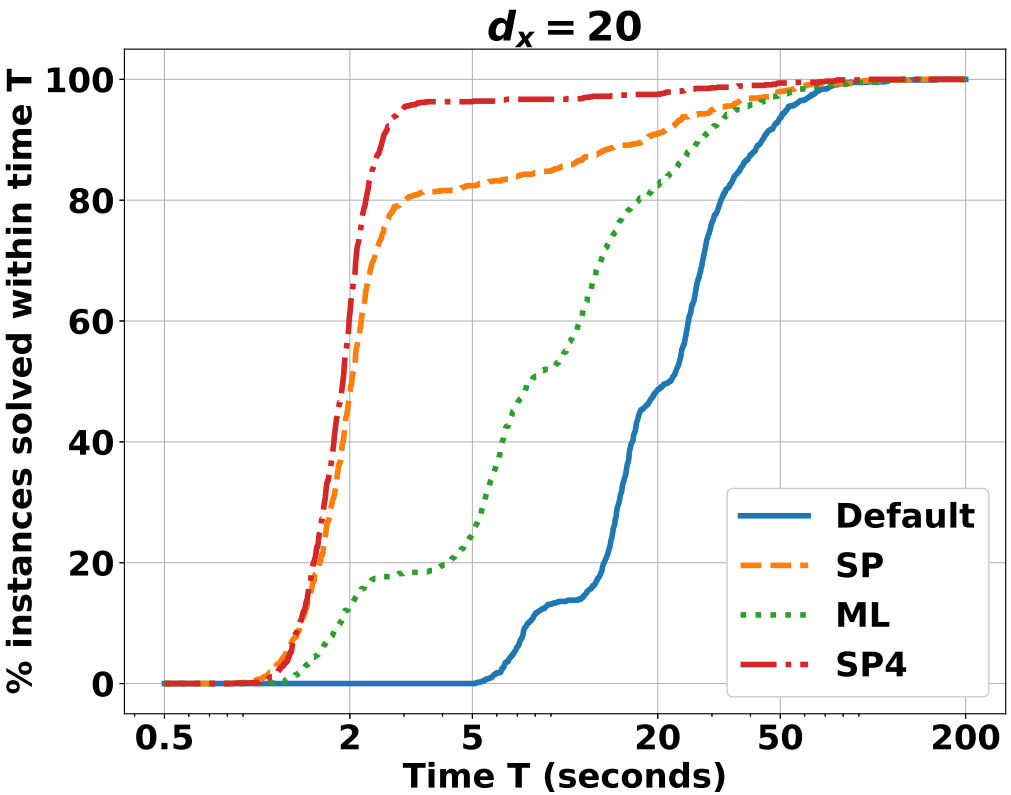

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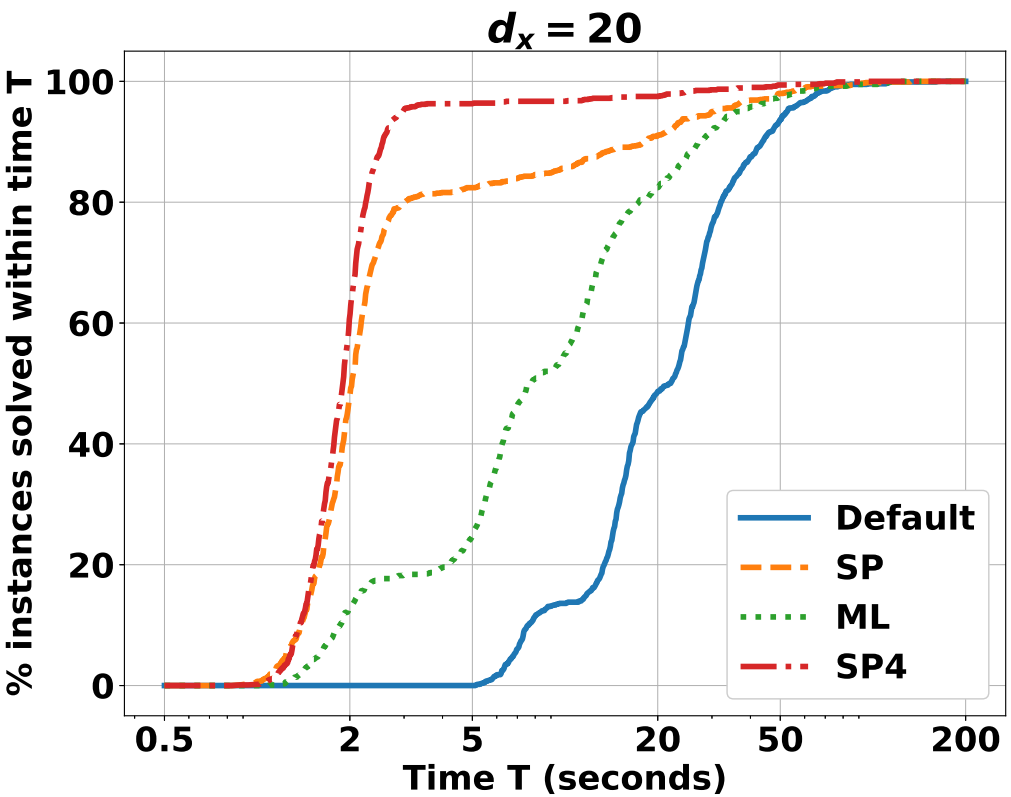

Speedup/ Slowdown	% SP Inst.	% ML Inst.
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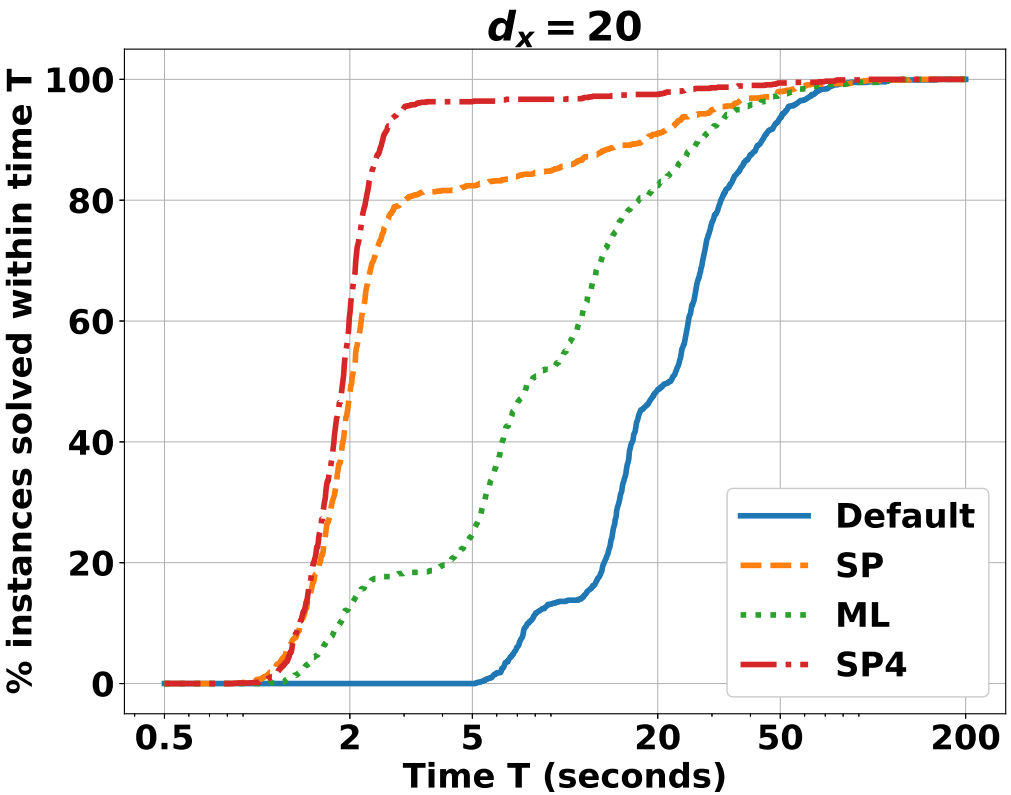

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Average Speedup (Shifted GM):

Alpine+SP: $5.1x$, Alpine+ML: $2.1x$

Alpine+SP4: $9x$, Alpine+ML4: $2.3x$

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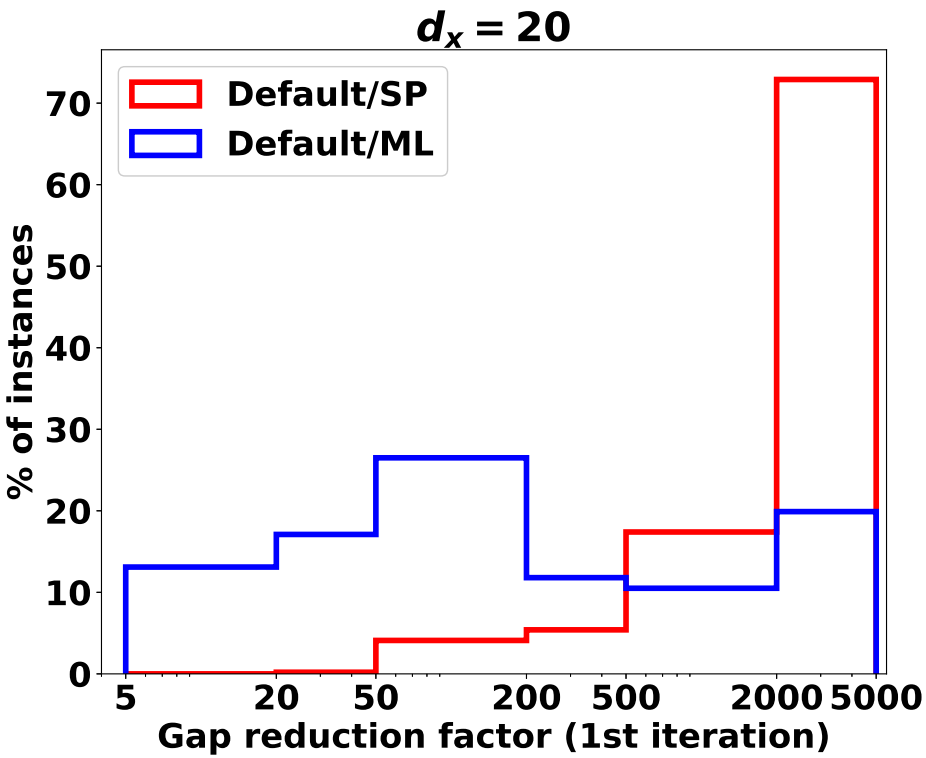

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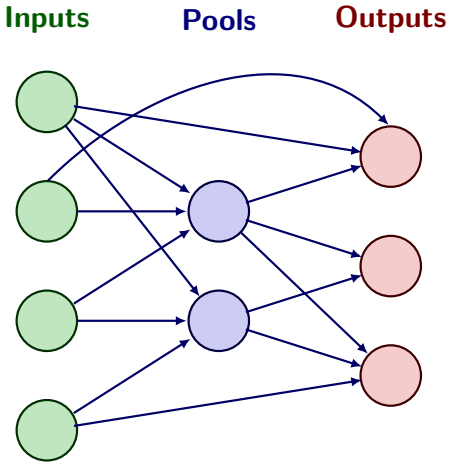

- 45 sources, 15 pools, 30 terminals, 1 quality (124/572 variables part. in 261 bilinear terms)
- 1000 random instances with θ = input qualities
- 2 SP points per variable (total 124×2)

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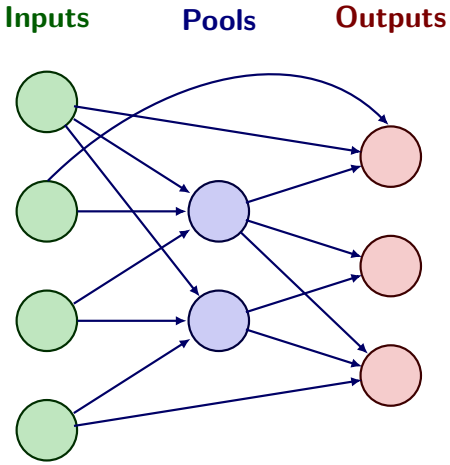

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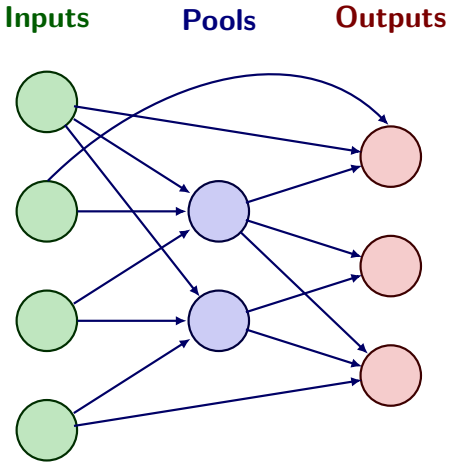

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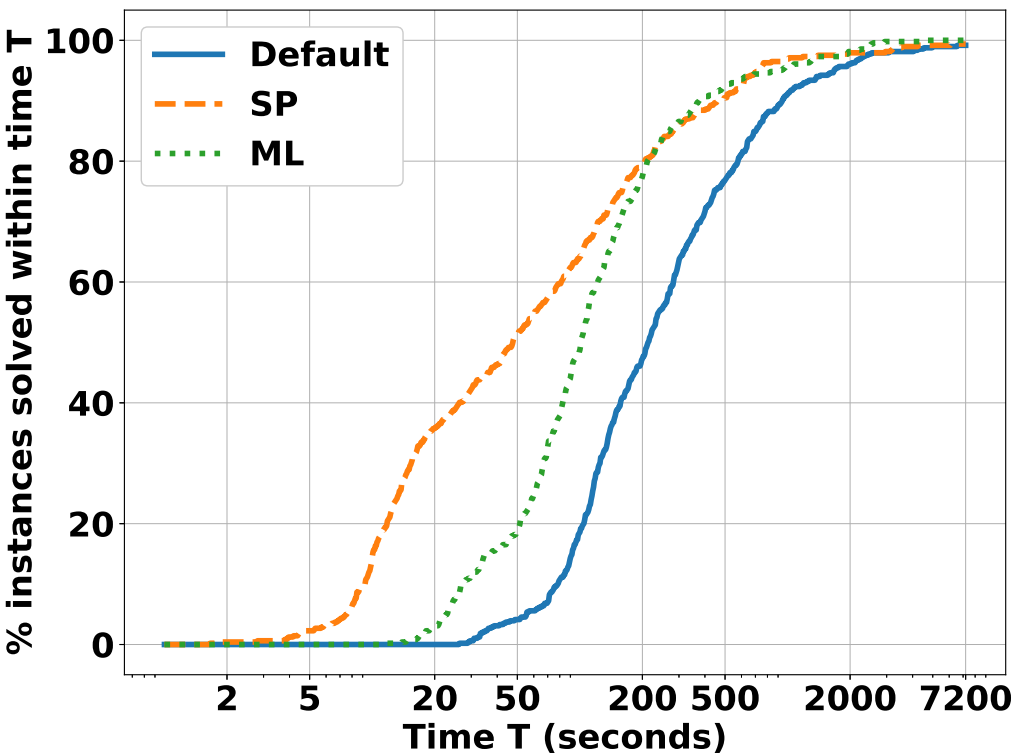

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Average Speedup (Shifted GM):

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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 $10x - 200x$)

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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

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ER-SAA

Numerical Study: Optimal Resource Allocation

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

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

$$\begin{aligned} Q(z, Y) := \min_{w, v \geq 0} \quad & d^{\mathsf{T}} w \\ \text{s.t.} \quad & \sum_{j \in \mathcal{J}} v_{ij} \leq z_i, \quad \forall i \in \mathcal{I}, \\ & \sum_{i \in \mathcal{I}} \mu_{ij} v_{ij} + w_j \geq Y_j, \quad \forall j \in \mathcal{J}. \end{aligned}$$

- 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 ζ_n
  - Approach 2: Use the data $\mathcal{D}_n$ to choose ζ_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

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

where $\mathcal{Z} := \left\{ z \in \mathbb{R}^{d_z}_+ : \sum_i z_i = 1 \right\}$.

- z_i: fraction of capital invested in asset i
- Y_i: uncertain net return of asset i
- $\mathrm{CVaR}_\beta \approx$ 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 $\bar{\varepsilon}_j \sim \mathcal{N}(0, 0.025j)$, $\omega \sim \mathcal{N}(0, 0.02)$, $\theta \in \{0.5, 1, 2\}$, $\dim(X) \in \{10, 100\}$

- 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 η_j are zero-mean errors

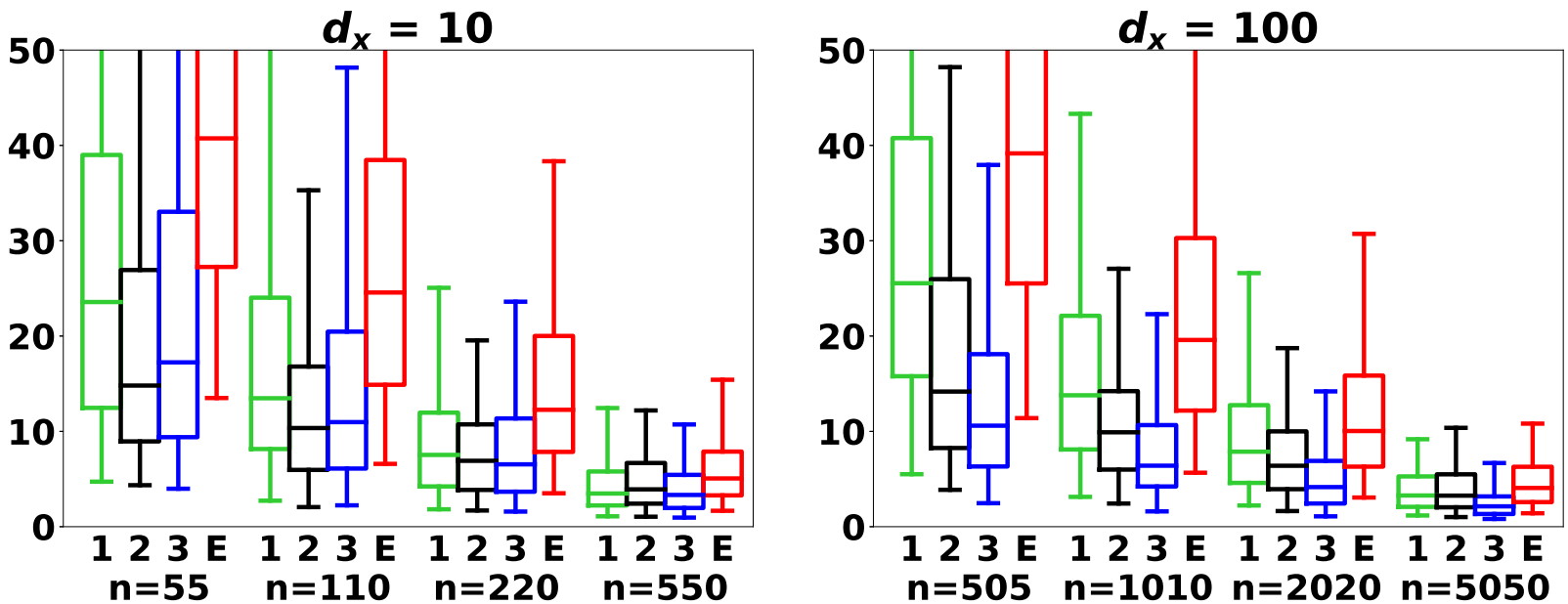
- Estimate optimality gap of solutions $\hat{z}_n^{ER}(x)$ and $\hat{z}_n^{DRO}(x)$

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

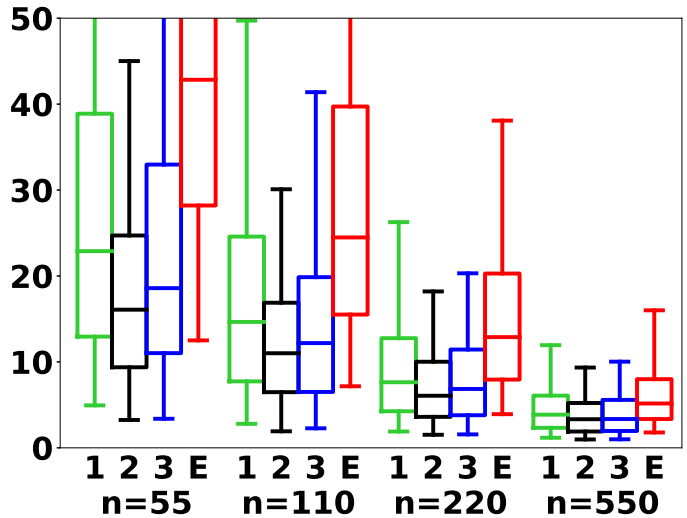
Whiskers: 5 and 95 percentiles

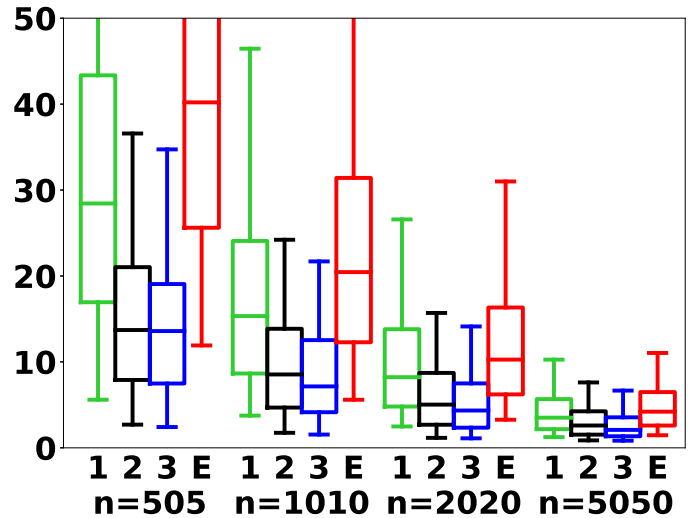
Sample sizes: $\{5, 10, 20, 50\} \times (\dim(X) + 1)$

Results with OLS and Misspecified Model Class ($\theta \neq 1$)

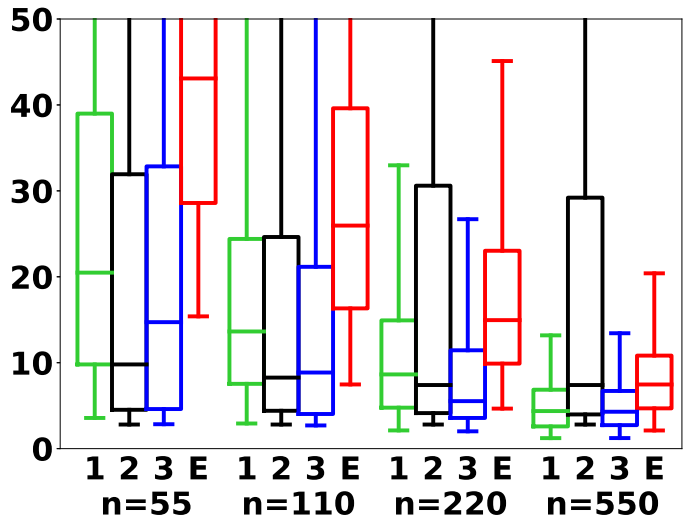
$\mathbf{d_x = 10}$ $\mathbf{d_x = 100}$

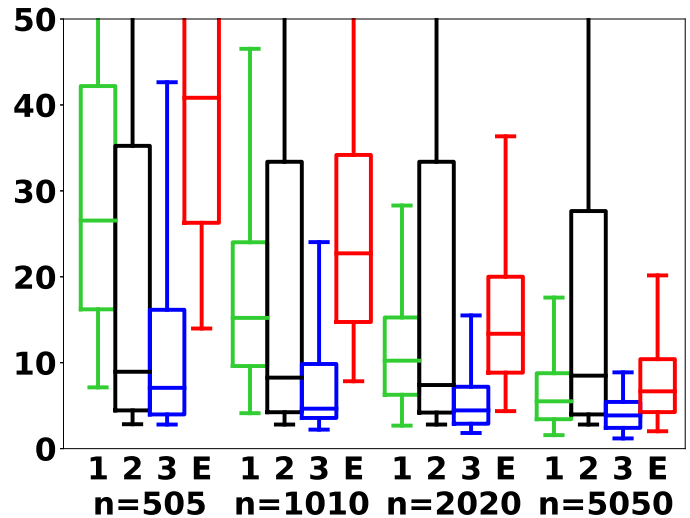
$\theta = 0.5$





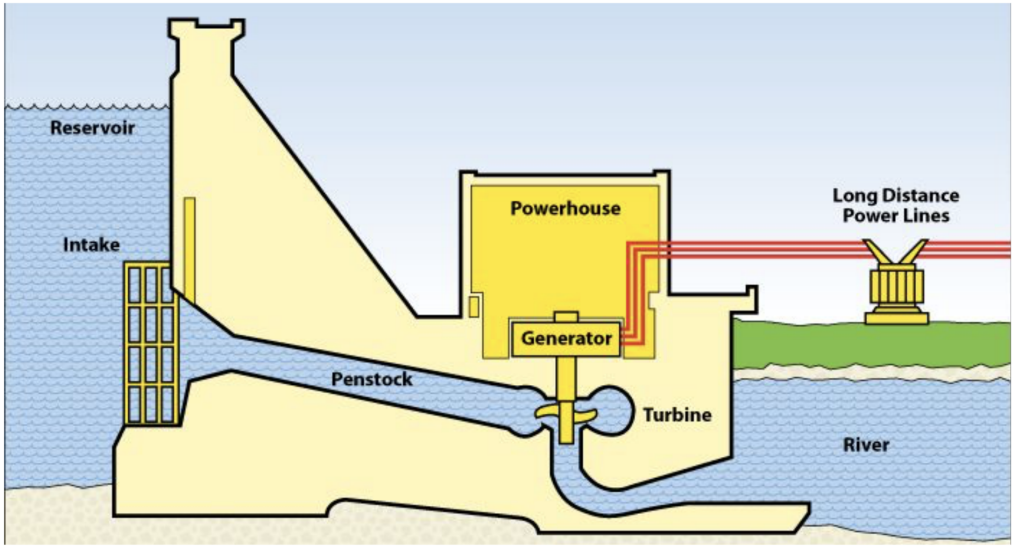
$\theta = 2$





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 :

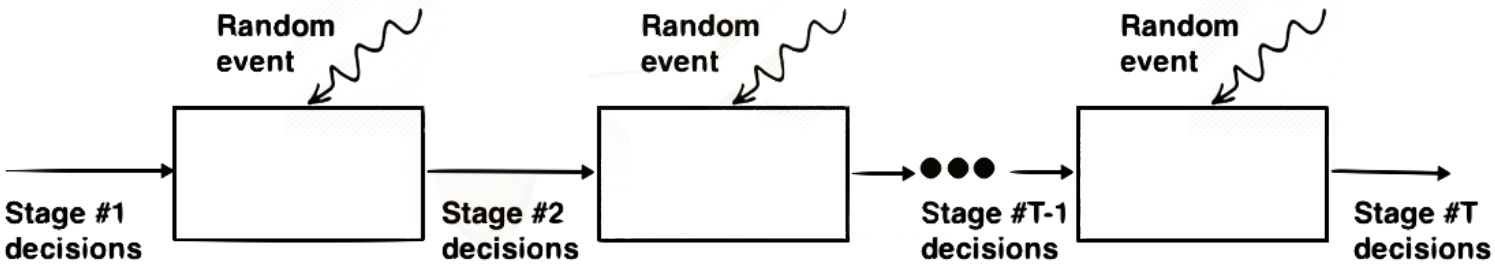
reservoir volume increase = rainfall - generation

thermal + hydro generation = demand

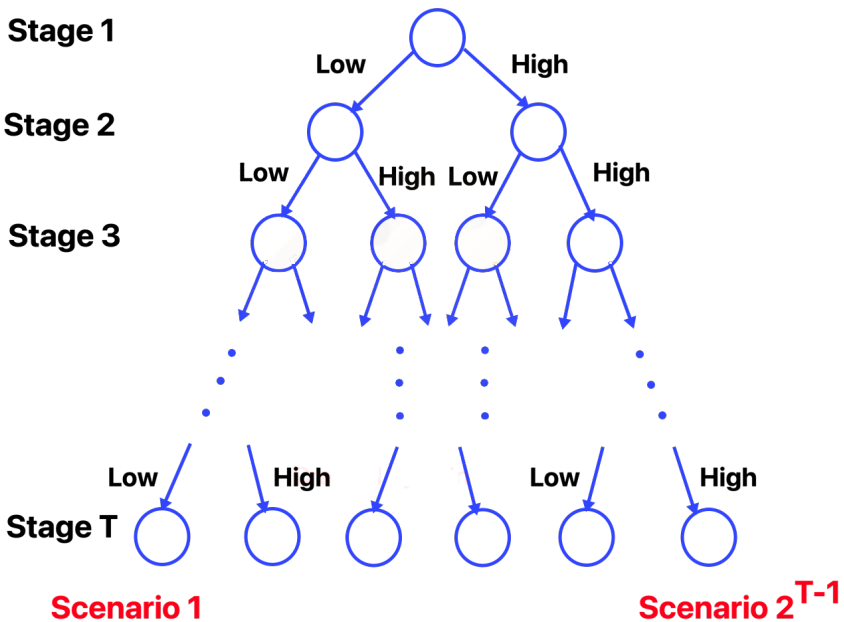
bounds on reservoir height, generation amounts

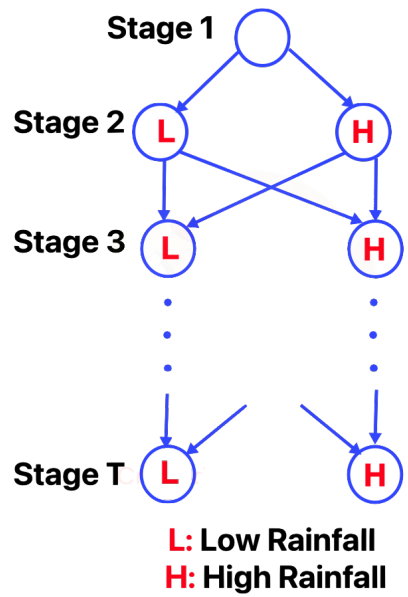
- Uncertain rainfall at each time stage t

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

$$V_t(x_{t-1}, \xi_{[t]}) := \min_{x_t \in X_t(x_{t-1}, \xi_t)} f_t(x_t, \xi_t) + \mathbb{E}\left[V_{t+1}(x_t, \xi_{[t+1]}) \mid \xi_{[t]}\right], \quad t \in [T-1],$$
$$V_T(x_{T-1}, \xi_{[T]}) := \min_{x_T \in X_T(x_{T-1}, \xi_T)} f_T(x_T, \xi_T) \qquad \text{(MSSP)}$$

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

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

We deal with multi-stage stochastic LPs, where

- $f_t(x_t, \xi_t) := c_t^\top x_t$
- $X_t(x_{t-1}, \xi_t) := \left\{x_t \in \mathbb{R}_+^{n_t} : B_t(\xi_t)x_{t-1} + A_t x_t = h_t(\xi_t)\right\}$

K., Ho-Nguyen, and Luedtke. Data-driven multistage stochastic optimization on time series. Working Paper

Problem Setup

- Given historical data from a *single trajectory* of $\{\xi_t\}$

$$\mathcal{D}_n := \left\{\tilde{\xi}_s, \tilde{\xi}_{s+1}, \cdots, \tilde{\xi}_{s+n}\right\}$$

- Want to solve

$$V_1(x_0, \xi_1) := \min_{x_1 \in X_1(x_0, \xi_1)} f_1(x_1, \xi_1) + \mathbb{E}\left[V_2(x_1, \xi_2) \mid \xi_1\right],$$

where

$$V_t(x_{t-1}, \xi_t) := \min_{x_t \in X_t(x_{t-1}, \xi_t)} f_t(x_t, \xi_t) + \mathbb{E}\left[V_{t+1}(x_t, \xi_{t+1}) \mid \xi_t\right], \quad t \in [T-1],$$
$$V_T(x_{T-1}, \xi_T) := \min_{x_T \in X_T(x_{T-1}, \xi_T)} f_T(x_T, \xi_T).$$

- 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*

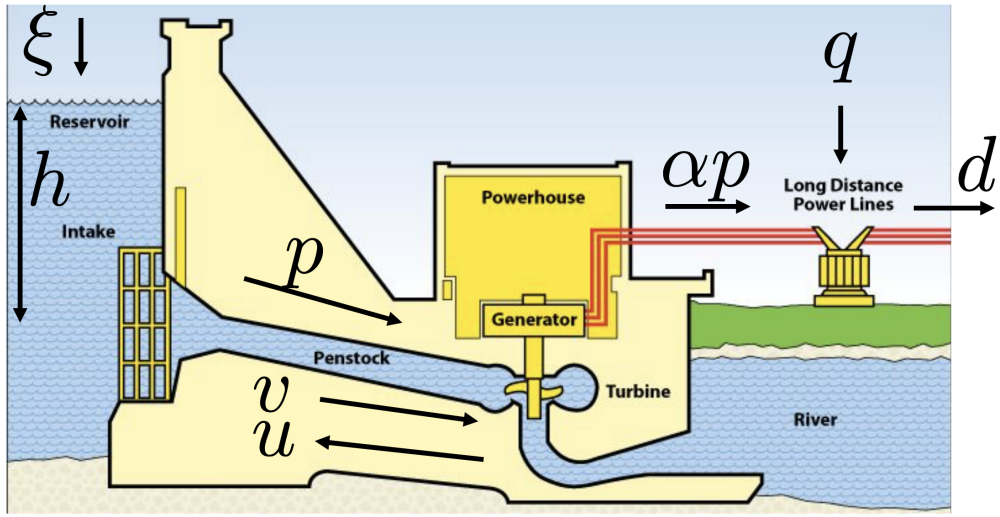
$$\hat{\varepsilon}_n^i := [\hat{Q}_n(\tilde{\xi}_{s+i-1})]^{-1}\big(\tilde{\xi}_{s+i} - \hat{f}_n(\tilde{\xi}_{s+i-1})\big), \quad i \in [n]$$

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

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

- 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



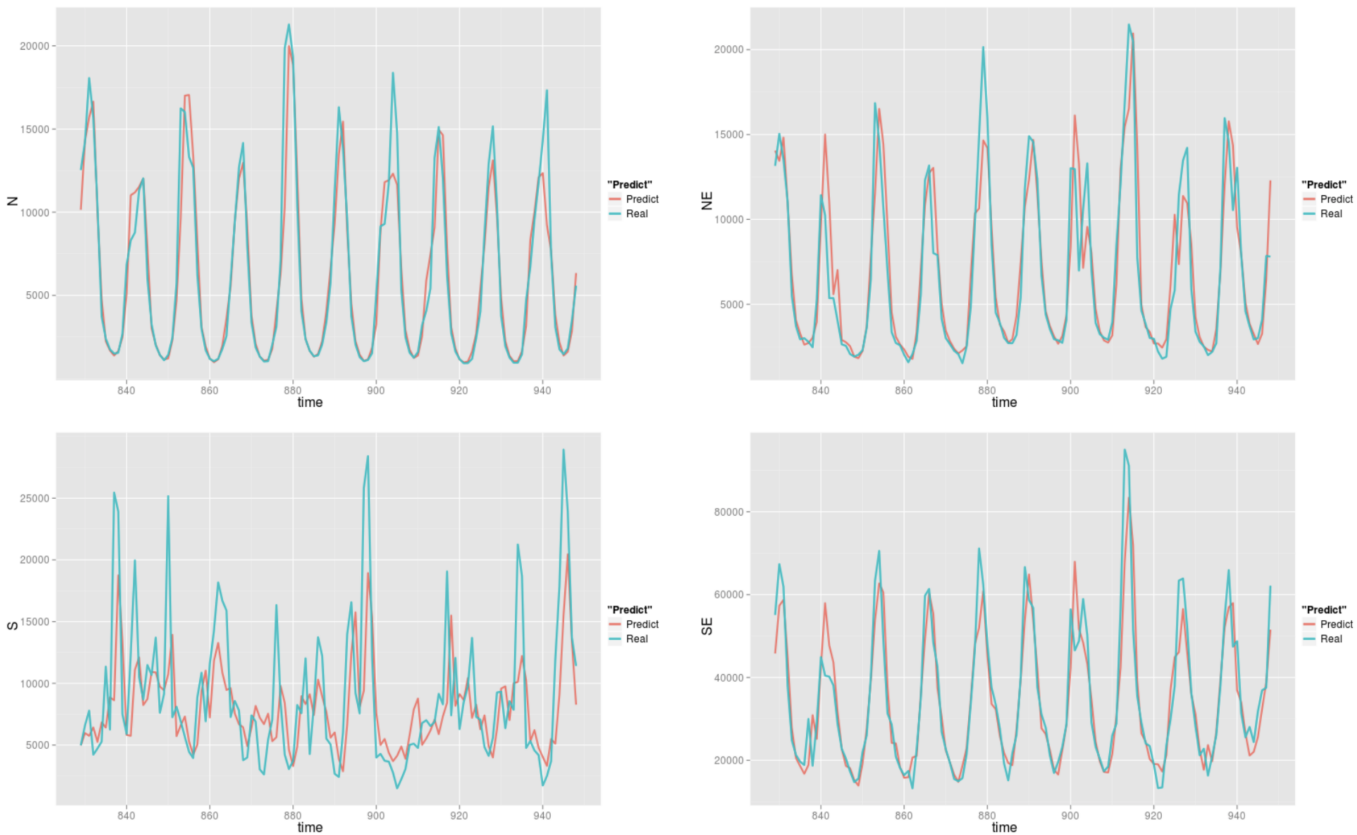
- Decisions z_t: Hydrothermal & natural gas generation, spillage
- Random vector ξ: Amount of rainfall

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



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

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

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

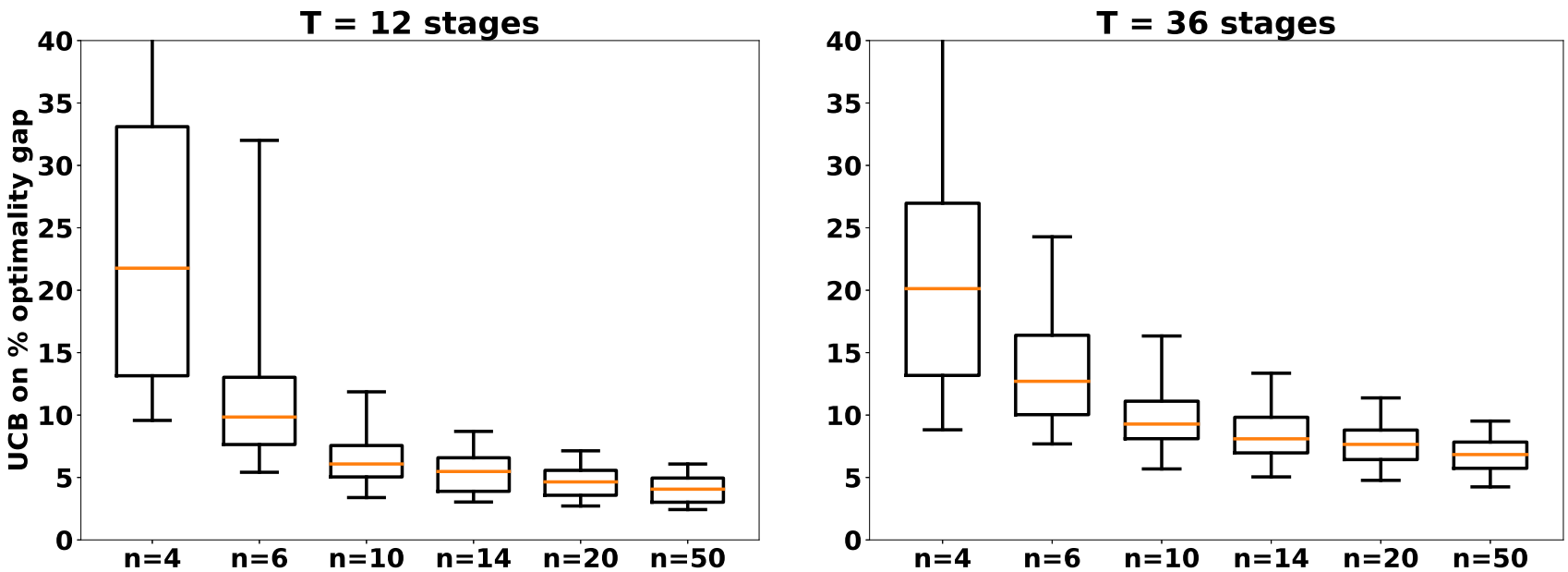
Use these to estimate samples of the errors ε_t

- 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 $\Longrightarrow$ closer to optimal



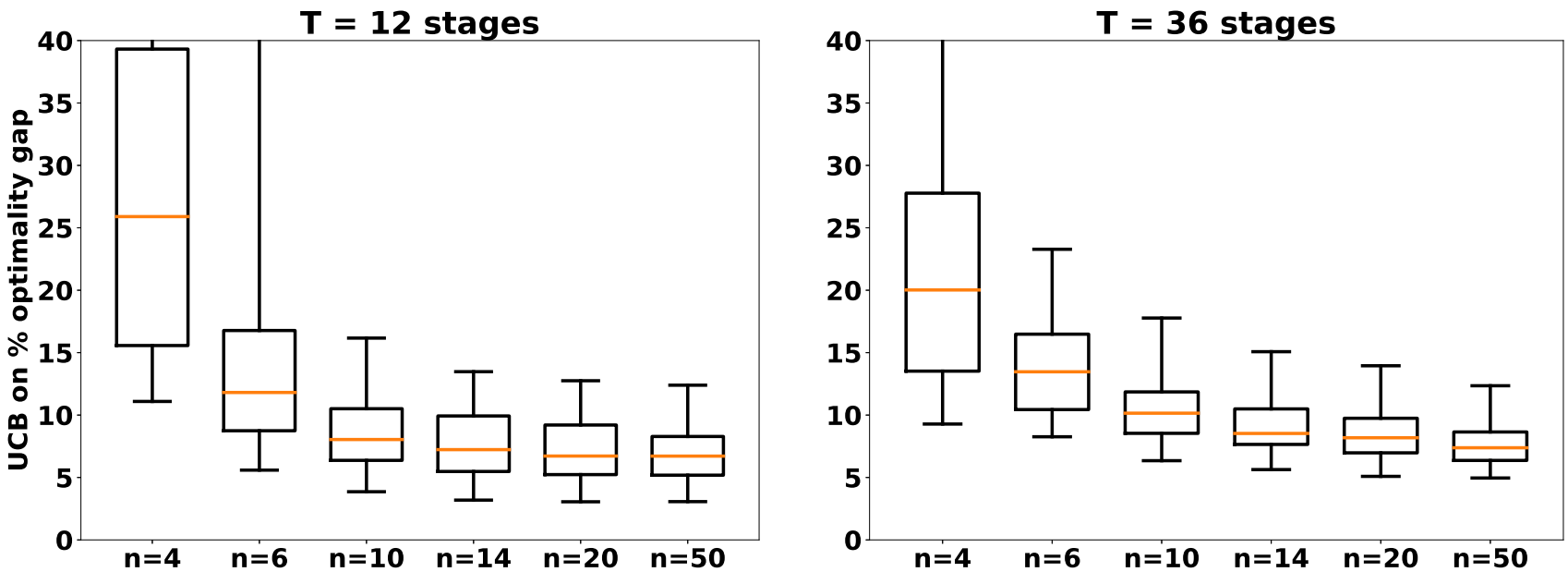
n: number of historical samples *per month*

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: $\xi_t = \alpha_t^* + \beta_t^* \xi_{t-1} + \varepsilon_t$

Lower y-axis value $\Longrightarrow$ 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 θ

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

- Generate 1000 training samples $\{\theta^i\}$ of problem parameters θ
- 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 $\bar{\theta}$

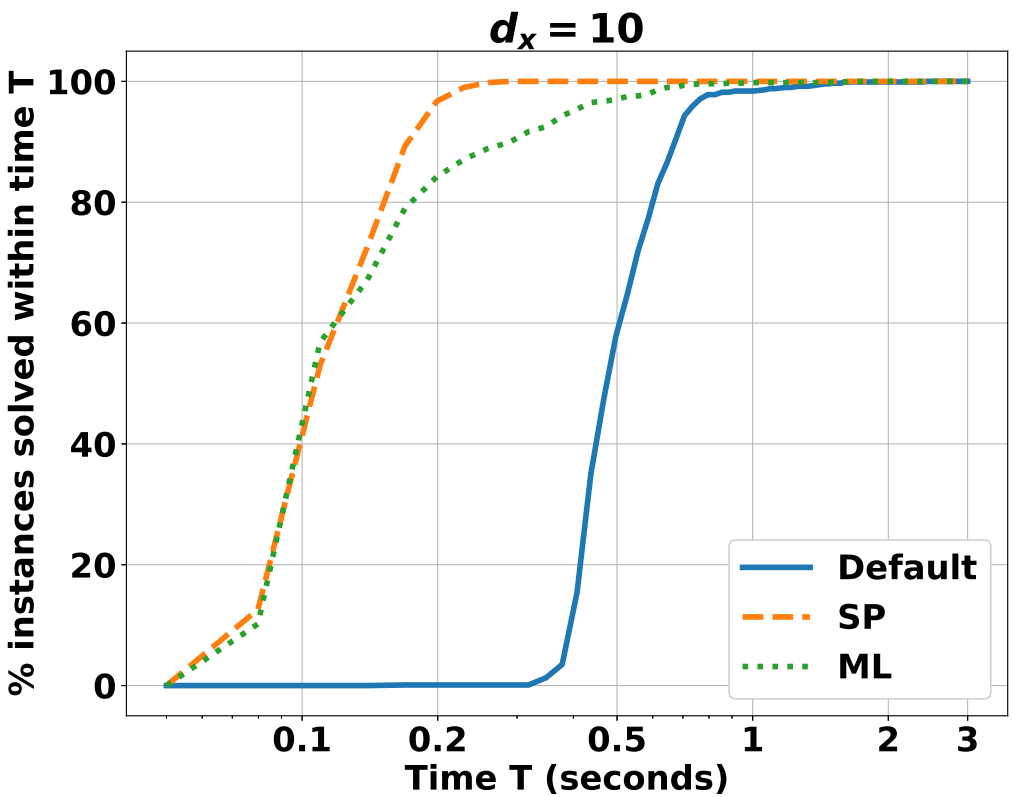
Use Scikit-learn's AdaBoostRegressor to train Regression Trees with max_depth $= 25$, num_estimators $= 1000$ (no tuning!)

- Features for training and prediction:
  - Parameter θ
  - 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 θ
- For each instance, determine 2 optimal partitioning points per variable by solving a max-min problem
- Eliminate optimal partitioning points that aren't useful



Speedup/ Slowdown	% SP Inst.	% ML Inst.
$1x - 2x$	1.1	7.7
$2x - 3x$	10.2	11.4
$3x - 5x$	47.4	38.5
$5x - 10x$	40.1	40.0
$> 10x$	1.2	0.1
$0.5x - 1x$	—	2.1
$< 0.5x$	—	0.2

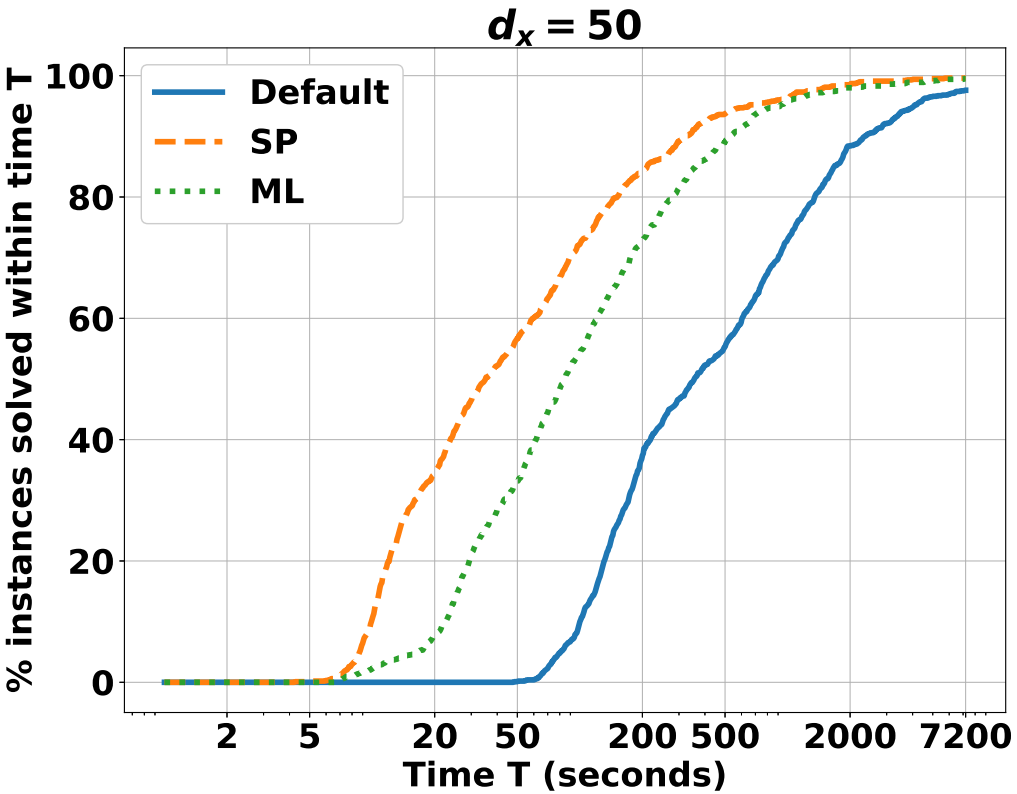
Average Speedup (Shifted GM):

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 θ
- 2 partitioning points per variable for each instance
- Eliminate partitioning points that aren't useful



Speedup/ Slowdown	% SP Inst.	% ML Inst.
$1x - 5x$	25.7	49.3
$5x - 10x$	26.3	25.3
$10x - 20x$	24.3	13.7
$20x - 50x$	14.9	5.4
$> 50x$	6.9	0.8
$0.5x - 1x$	1.5	4.8
$< 0.5x$	0.4	0.7

Average Speedup (Shifted GM):

Alpine+SP: $8.1x$, Alpine+ML: $4.2x$