A Unified Approach to Mixed-Integer Optimization: Nonlinear Formulations and Scalable Algorithms

Ryan Cory-Wright

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ORC, Massachusetts Institute of Technology
Joint work with Dimitris Bertsimas and Jean Pauphilet

Note: Jean is on the job market. He is giving talks on Tuesday (TA66), Wednesday (WC34).

Preprint available: ryancorywright.github.io

Motivation: A Tale of Two Problems

Best Subset Selection: Fit parsimonious model using at most k features

$$\min_{\boldsymbol{x} \in \mathbb{R}^p, \boldsymbol{z} \in \{0,1\}^p} \quad \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{x}\|_2^2 \text{ s.t.} \quad \sum_i z_i \leq k, -Mz_i \leq x_i \leq Mz_i, \forall i \in [p].$$

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Facility Location: Build facilities z_i and ship amount $X_{i,j}$ to node j

$$\begin{aligned}\min_{\boldsymbol{z}\in\{0,1\}^n} \ \min_{\boldsymbol{X}\in\mathbb{R}_+^{n\times m}} \quad & \langle \boldsymbol{c}, \boldsymbol{z}\rangle + \langle \boldsymbol{C}, \boldsymbol{X}\rangle \\ \text{s.t.} \quad & \sum_{j=1}^m X_{ij} \leq U_i,\ \forall i \in [n],\ \sum_{i=1}^n X_{ij} = d_j,\ \forall j \in [m], \\ & X_{ij} \leq U_i z_i,\ \forall i \in [n],\ \forall j \in [m].\end{aligned}$$

What do These Problems Have in Common?

- Two MIOs with big-M constraints between binary $\boldsymbol{z}$, continuous $\boldsymbol{x}$.
- MIO books (e.g. B.+Weismantel 2004) introduce problems this way *by default*.

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- Two MIOs with big-M constraints between binary $\boldsymbol{z}$, continuous $\boldsymbol{x}$.
- MIO books (e.g. B.+Weismantel 2004) introduce problems this way *by default*.
- But... big-M formulations actually **reformulations** of true problems!

The True Formulations

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True formulations are MIOs with logical structure: $x = 0$ *if* $z = 0$.

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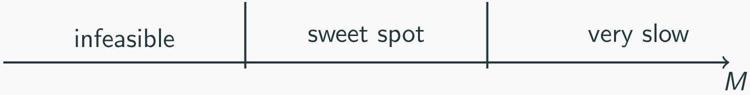

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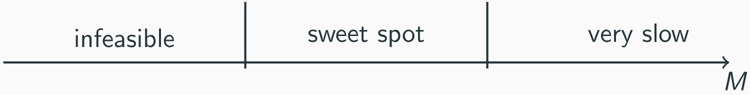

Big-M constraints often inhibit scalability. Alternatives are needed.

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Logical on/off structure appears in many important problems!

Central problems in optimization/statistics have logical relations between continuous variables $\boldsymbol{x}$, binary variables $\boldsymbol{z}$: $\boldsymbol{x} = \mathbf{0}$ *if* $\boldsymbol{z} = \mathbf{0}$.

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- Many others: **Sparse Portfolio Selection, Network Design, Unit Commitment, Scheduling, Binary Quadratic, Sparse PCA**.

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- We show that adding a $\frac{1}{2\gamma}\|\boldsymbol{x}\|_2^2$ **ridge regularizer** to the objective is a viable and often more scalable alternative to big-M.

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- We obtain provably **near-optimal solutions in polynomial time** by solving a Boolean relaxation efficiently.
- Our approach **is scalable**: it solves sparse regression problems with $100,000$s of covariates, sparse portfolio selection problems with 1000s of securities, network design problems with 100s of nodes.

The Unified Framework

A Mixed-Integer Nonlinear Program With Logical Constraints

$$\min_{\boldsymbol{z}\in\mathcal{Z},\ \boldsymbol{x}\in\mathbb{R}^n} \boldsymbol{c}^\top \boldsymbol{z} + \underbrace{g(\boldsymbol{x})}_{\text{convex function}} + \underbrace{\Omega(\boldsymbol{x})}_{\text{regularizer}} \text{ s.t. } \underbrace{x_i = 0 \text{ if } z_i = 0}_{\text{logical constraint}},\ \forall i,$$

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- We model convex constraints $\boldsymbol{x} \in \mathcal{X}$ via $g(\boldsymbol{x}) = +\infty$ if $\boldsymbol{x} \notin \mathcal{X}$.
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    1. A big-M penalty: $\Omega(\boldsymbol{x}) = 0$ if $\|\boldsymbol{x}\|_\infty \le M$ and $+\infty$ otherwise.
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All six problems on the second slide fit into this framework!

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- Allows us to solve all six problems using the same piece of code.

Fitting Facility Location Within Our Framework

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Simplifying the Problem

We rewrite the problem as

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which proves $f(z)$ is convex!

So What?

The Outer-Approximation Method

Our saddle-point representation:

$$\min_{\boldsymbol{z} \in \mathcal{Z}} f(\boldsymbol{z}) = \min_{\boldsymbol{z} \in \mathcal{Z}} \max_{\boldsymbol{\alpha}} \boldsymbol{c}^\top \boldsymbol{z} + h(\boldsymbol{\alpha}) - \sum_i z_i \Omega^\star(\alpha_i)$$

lends itself to a tractable outer-approximation method.

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- Iteratively adding cuts, minimizing piecewise linear underestimator in Julia/CPLEX minimizes $f(\boldsymbol{z})$. Using Branch-and-Cut with lazy constraints solves entire problem using one branch-and-bound tree.
- As will see in numerical results, solves very large-scale problems.

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We solve the problem

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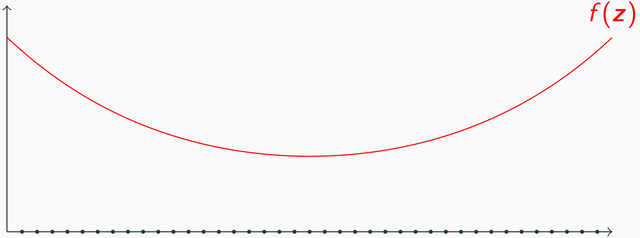
by iteratively minimizing a piecewise linear underestimator of f.



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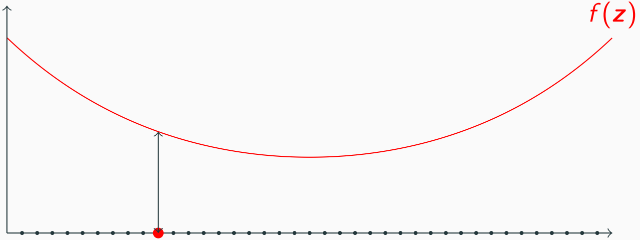

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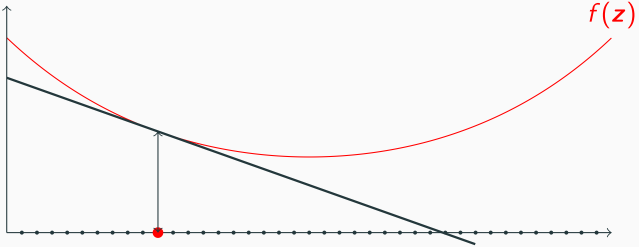

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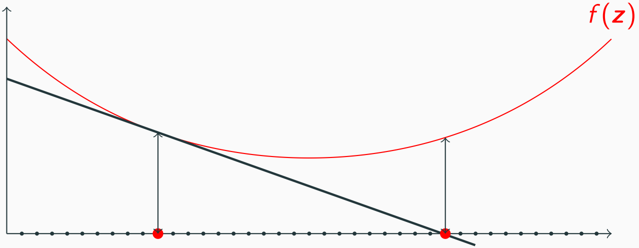

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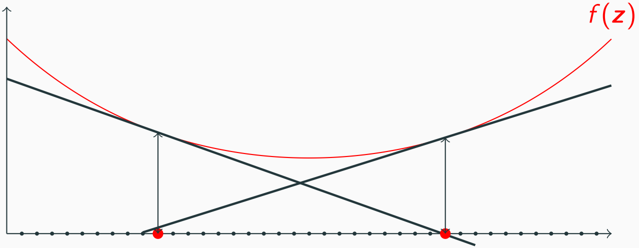

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We solve the problem

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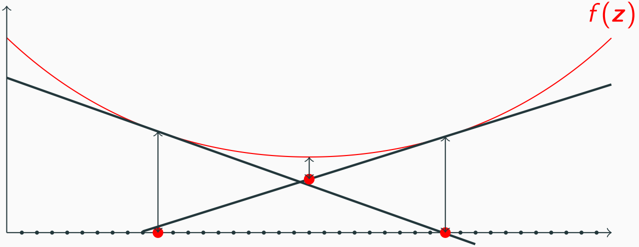

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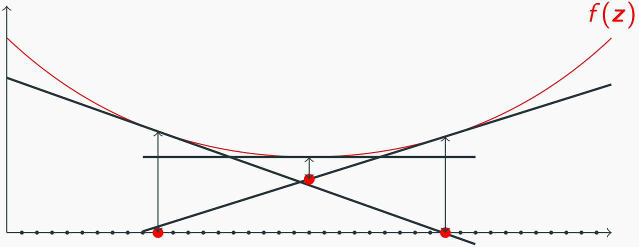

A Boolean Relaxation

$$\min_{\boldsymbol{z}\in\mathrm{Conv}(\mathcal{Z})} \max_{\boldsymbol{\alpha}} \; \boldsymbol{c}^\top \boldsymbol{z} + h(\boldsymbol{\alpha}) - \sum_i z_i \Omega^\star(\alpha_i)$$

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- Randomly rounding relaxation $\boldsymbol{z}^\star$ according to $z_i \sim \mathrm{Bernoulli}(z_i^\star)$ gives a Boolean vector $\boldsymbol{z}$. How good is it?
- Let $\boldsymbol{z}$ be a random rounding of $\boldsymbol{z}^\star$. Then,

$$0 \leq f(\boldsymbol{z}) - f(\boldsymbol{z}^\star) \leq \epsilon$$

with probability at least

$$1 - |\mathcal{R}| \exp\left(\frac{-\epsilon^2}{\kappa}\right)$$

  - $|\mathcal{R}|$ is number of strictly fractional entries in $\boldsymbol{z}^\star$.
  - κ is a function of $|\mathcal{R}|$, problem data.

How does the approach perform on real data?

Sparse Empirical Risk Minimization Scalability

- For regression $f(\boldsymbol{z})$ is closed form, scales to $100,000$s of features.
- For classification, $f(\boldsymbol{z})$ is cheap, scales to $10,000$s of features.
- Outer-approximation algorithm is more accurate than ElasticNet, MCP, SCAD, and runtimes are comparable to Lasso.
- Code available: github.com/jeanpauphilet.

Sparse Portfolio Selection Scalability

Solves sparse portfolio selection problems with $1,000$s of securities.

Reference	Solution method	Size (no. securities)
Frangioni and Gentile ($'09$)	Perspective cut+SDP	400
Bonami and Lejeune ($'09$)	Nonlinear Branch-and-Bound	200
Gao and Li ($'13$)	SOCP relaxation Branch-and-Bound	300
Cui et al. ($'13$)	SOCP relaxation Branch-and-Bound	300
Zheng et. al. ($'14$)	SDP Branch-and-Bound	400
Frangioni et. al. ($'16$)	Aprox. Proj. Perspective Cut	400
Bertsimas and C-W ($'18$)	OA with γ-regularization	$3,200$

Network Design Scalability

- $f(\boldsymbol{z})$ obtained by solving a quadratic program.
- Approach solves problems with 100s of nodes.
- Objective value 5% better than CPLEX for small problems, 40% better for large problems.

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Main Messages and Highlights

- Don't feel married to big-M! We provide a **non-linear alternative** which often scales as well or better: substituting xz for x and adding a ridge regularizer.
- By using strong duality, we derive a saddle-point reformulation, which is **exactly** solvable via an outer-approximation procedure.
- Our approach: outer-approximation+warm-start+random rounding **is scalable**.

Thanks for listening!

Questions?

Preprint available at: ryancorywright.github.io

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