Tutorial

Solving L_0-norm Problems via Mixed-Integer Optimization

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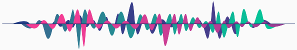
MIND and SODA team seminar
October 10th, 2023
Inria Paris Saclay, France

Sparse Optimization

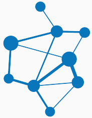
Two goals, one problem

Minimize a function $\xleftrightarrow{\textbf{Sparse optimization}}$ **Sparse solution**



Signal processing

Machine learning



Network design

And many others

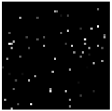
Signal processing

Compressive sensing

Linear measurement through $A \in \mathbb{R}^{m \times n}$

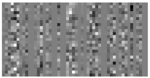
Sparse signal

$x \in \mathbb{R}^n$



Observation

$y \in \mathbb{R}^m$



Recover x from (A, y)

Find x **such that** $y \simeq Ax$

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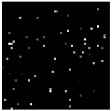

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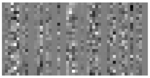

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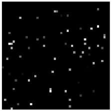

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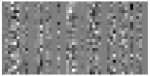

Recover x from (A, y)

Find x **sparse such that** $y \simeq Ax$

$m \ll n$: no unique solution

Machine learning

Heart disease dataset (LIBSVM)

Age	Sex	Cholesterol	Blood pressure	...	**Disease**
31	M	50.3 mg/dl	95 mm/hg	...	**No**
35	F	54.9 mg/dl	98 mm/hg	...	**Yes**
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Data ⟶ **Logistic regression** $\min_x \ \text{LogLoss}(x)$ ⟶ **Estimator**

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Involves all the features

Explainability and robustness issues

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Data → **Logistic regression** $\min_x \ \mathrm{LogLoss}(x)$ → **Estimator**

Force the use of only few features via sparsity in x

Involves all the features
Explainability and robustness issues

Finance

Portfolio selection problem

$$\begin{cases} \max & c^{\mathrm{T}}x - \frac{\sigma}{2}x^{\mathrm{T}}\Sigma x \\ \text{s.t.} & 1^{\mathrm{T}}x = 1 \\ & x \text{ is k-sparse} \end{cases}$$

x_i : proportion of investment in asset i

c_i : profit of asset i

$\Sigma_{i,j}$: covariance of assets i and j

k : diversification budget

Objective, constraint or both ?

Minimize a function $\xleftrightarrow{\textbf{Sparse optimization}}$ **Sparse solution**

Loss $F(x)$

Counting function $\|x\|_0$

Objective, constraint or both ?

Minimize a function $\xleftrightarrow{\textbf{Sparse optimization}}$ **Sparse solution**

Loss $F(\mathrm{x})$

Counting function $\|\mathrm{x}\|_0$

Constrainted version

$$\begin{cases} \min_{\mathrm{x}} & F(\mathrm{x}) \\ \text{s.t.} & \|\mathrm{x}\|_0 \leq s \end{cases}$$

Minimized version

$$\begin{cases} \min_{\mathrm{x}} & \|\mathrm{x}\|_0 \\ \text{s.t.} & F(\mathrm{x}) \leq \epsilon \end{cases}$$

Penalized version

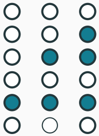
$$\min_{\mathrm{x}} F(\mathrm{x}) + \lambda \|\mathrm{x}\|_0$$

A bit of history

1990

Sparse
heuristics

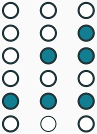
MP, OMP,
IHT and co.



A bit of history

1990 **2000**

Sparse heuristics



Formulation with ℓ_0-norm

RIP, NSP, EkR and co.

OMP

|||

ℓ_0-prob.

A bit of history

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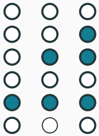


2000

Formulation with ℓ_0-norm

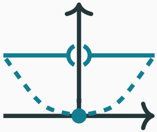
RIP, NSP, EkR and co.

OMP
|||
ℓ_0-prob.

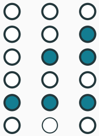
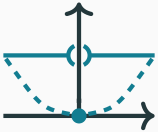
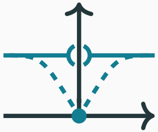
2005

Convex approx. of ℓ_0-norm

Lasso, Elastic-Net and co.

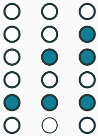


A bit of history

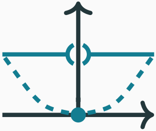
1990	2000	2005	2013
Sparse heuristics	Formulation with ℓ_0-norm	Convex approx. of ℓ_0-norm	Concave approx. of ℓ_0-norm
MP, OMP, IHT and co.	RIP, NSP, EkR and co.	Lasso, Elastic-Net and co.	SCAD, MCP CEL0 and co.
	OMP $\equiv$ ℓ_0-prob.		

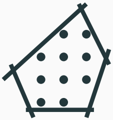
A bit of history

1990	2000	2005	2013	2016
Sparse heuristics	Formulation with ℓ_0-norm	Convex approx. of ℓ_0-norm	Concave approx. of ℓ_0-norm	Exact methods for ℓ_0-prob.
MP, OMP, IHT and co.	RIP, NSP, EkR and co.	Lasso, Elastic-Net and co.	SCAD, MCP CEL0 and co.	MIP, BnB CP and co.



OMP $\equiv$ ℓ_0-prob.





Why solving L0 problems ?

Solution quality

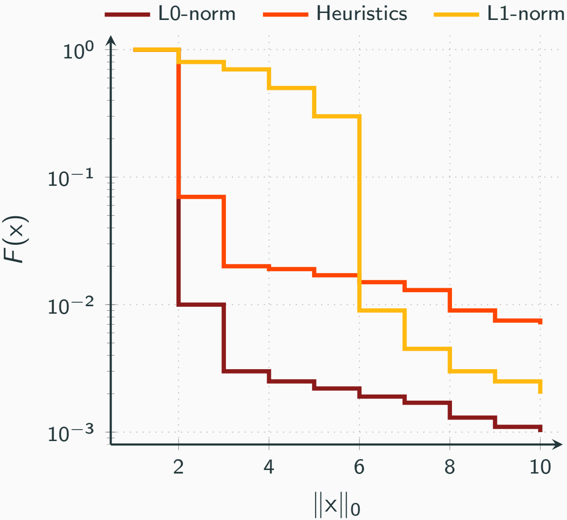
$\min_x F(x) + \lambda\|x\|_0$

vs

OMP heuristic

vs

$\min_x F(x) + \lambda\|x\|_1$



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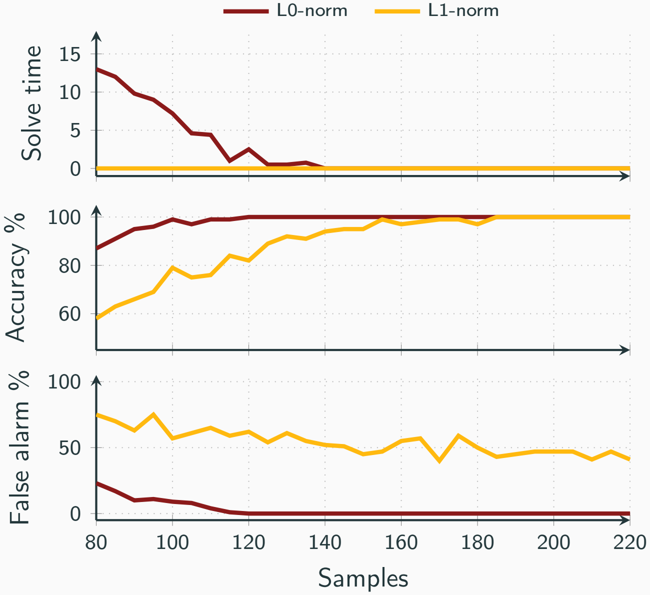

Sparse regression

$y = Ax^{\dagger} + \epsilon$

2.000 features

10 non-zeros in $x^{\dagger}$

20dB noise

D. Bertsimas and B. Van Parys, Sparse High-Dimensional Regression: Exact Scalable Algorithms and Phase Transitions

Mixed-Integer Optimization

Handeling the L0-norm with MIO tools

Problem

$\min_x F(x) + \lambda \|x\|_0$

$\downarrow$ $\boxed{\text{Solver}}$

Solution

Handeling the L0-norm with MIO tools

Problem

$\min_{x} F(x) + \lambda\|x\|_0$

Solver

Solution

Non-linear, non-convex,
non-smooth, NP-hard, ...

😵

Handeling the L0-norm with MIO tools

Problem

$\min_x F(x) + \lambda \|x\|_0$

Solver

Solution

Non-linear, non-convex,
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😵

The ℓ_0-norm counts the number of non-zeros
$\|x\|_0 = \mathrm{card}(\{i \mid x_i \neq 0\})$

It sums the entries of the binary vector z satisfying some logical relation with x

We have tools to deal with such binary vectors in MIO !

Problem formulation

Linearizing the ℓ_0-norm

Let $\mathrm{x} \in \mathrm{R}^n$ and $\mathrm{z} \in \mathrm{B}^n$ such that $x_i = 0 \iff z_i = 0$, then $\|\mathrm{x}\|_0 = 1^{\mathrm{T}}\mathrm{z}$.

Problem formulation

Linearizing the ℓ_0-norm

Let $\mathrm{x} \in \mathrm{R}^n$ and $\mathrm{z} \in \mathrm{B}^n$ such that $x_i = 0 \iff z_i = 0$, then $\|\mathrm{x}\|_0 = 1^{\mathrm{T}}\mathrm{z}$.

$$\min_{\mathrm{x},\mathrm{z}} F(\mathrm{x}) + \lambda 1^{\mathrm{T}}\mathrm{z} + H(\mathrm{x}, \mathrm{z})$$

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$$\min_{x,z} F(x) + \lambda 1^{\mathrm{T}} z + H(x, z)$$

Big-M

$$\begin{cases} \min_{x,z} & F(x) + \lambda 1^{\mathrm{T}} z \\ \text{s.t.} & -Mz \leq x \leq Mz \\ & x \in R^n, \; z \in B^n \end{cases}$$

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L2-norm

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Pros

- ✓ Fit the MIP formalism
- ✓ Available tools and methods
- ✓ Tailored solvers

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- ✗ Mostly commercial solvers
- ✗ Unable to exploit sparsity
- ✗ Not numerically efficient

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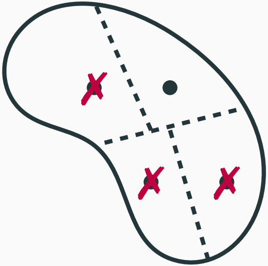
We need specialized methods able to exploit the structure !

Specialized Solution Methods

Branch-and-Bound algorithms

Branch-and-Bound

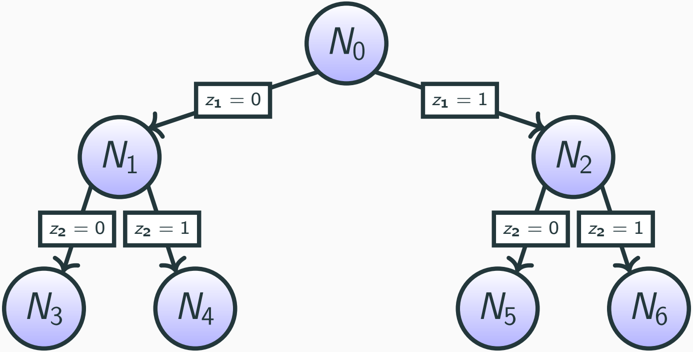
"Enumerate all candidate solutions and discard sub-optimal ones."



Main principles

Branching:	Divide the search space
Bounding:	Test whether a region can contain optimal solutions
Pruning:	Discard regions without optimal solutions

Tree exploration



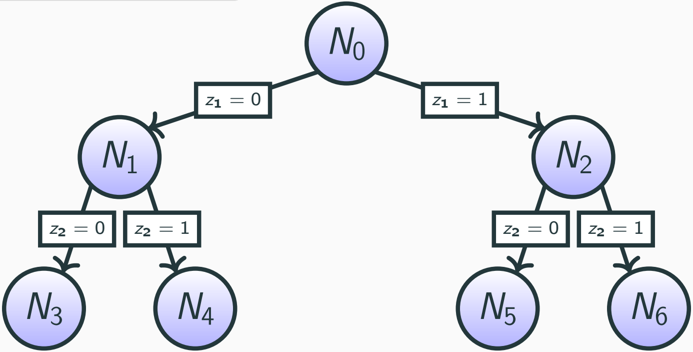
Tree exploration

Observation

If z is fixed, then

$$\min_{x,z} F(x) + \lambda 1^{T} z + H(x, z)$$

is fairly easy to solve.



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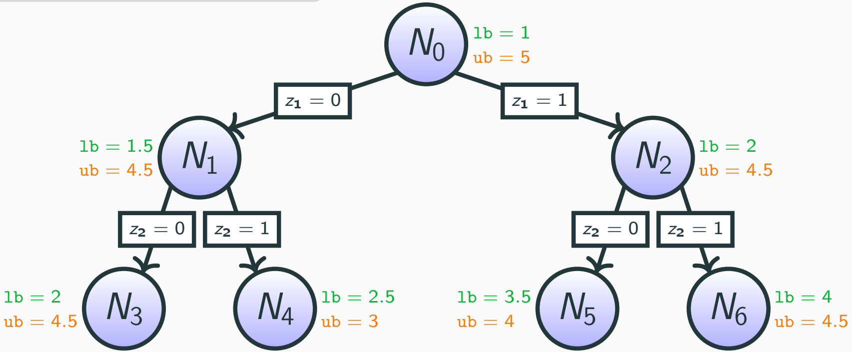

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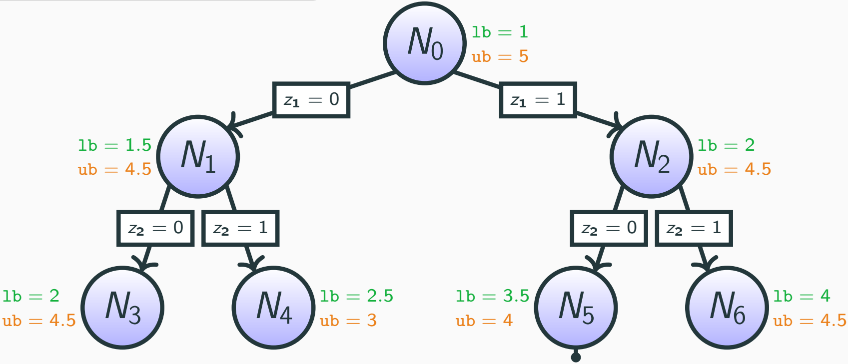

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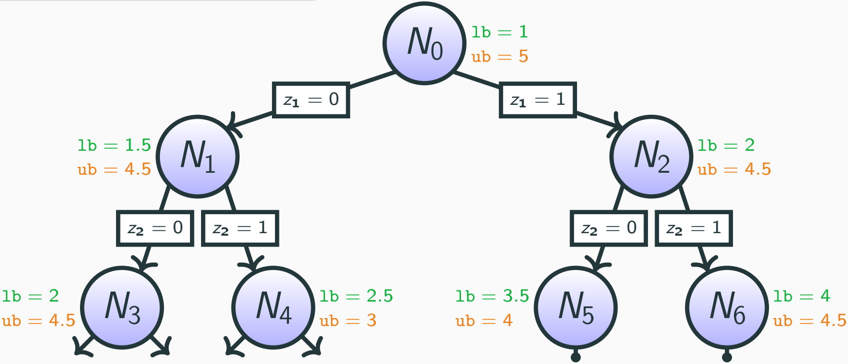

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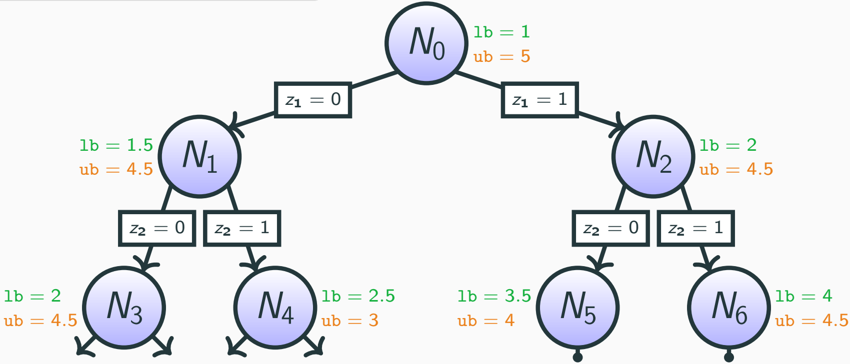

All nodes explored or pruned $\longrightarrow$ Problem solved

$(\mathcal{S}_0, \mathcal{S}_1)$

Node problem

The problem at node $\nu = (\mathcal{S}_0, \mathcal{S}_1)$ where $\mathcal{S}_0$ and $\mathcal{S}_1$ are the indices of z fixed to zero and one reads

$$p^{\nu} = \begin{cases} \min_{\mathrm{x},\mathrm{z}} & F(\mathrm{x}) + \lambda \mathbf{1}^{\mathrm{T}} \mathrm{z} + H(\mathrm{x}, \mathrm{z}) \\ \text{s.t.} & \mathrm{z}_{\mathcal{S}_0} = 0, \; \mathrm{z}_{\mathcal{S}_1} = 1 \end{cases}$$

Node processing

$(\mathcal{S}_0, \mathcal{S}_1)$

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Find some lower bound on p^ν

Find some upper bound on p^ν

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Find some upper bound on p^ν

Upper bounding

- We just need a feasible solution
- Fix entries that are still free to zero
- Optimize the resulting problem

Node processing

$(\mathcal{S}_0, \mathcal{S}_1)$

Node problem

The problem at node $\nu = (\mathcal{S}_0, \mathcal{S}_1)$ where $\mathcal{S}_0$ and $\mathcal{S}_1$ are the indices of z fixed to zero and one reads

$$p^\nu = \begin{cases} \min_{\mathrm{x},\mathrm{z}} & F(\mathrm{x}) + \lambda \mathbf{1}^{\mathrm{T}}\mathrm{z} + H(\mathrm{x}, \mathrm{z}) \\ \text{s.t.} & \mathrm{z}_{\mathcal{S}_0} = 0,\ \mathrm{z}_{\mathcal{S}_1} = 1 \end{cases}$$

Find some lower bound on p^ν

Find some upper bound on p^ν

Upper bounding

- We just need a feasible solution
- Fix entries that are still free to zero
- Optimize the resulting problem

Easy to solve

Upper-bounding problem

$$\min_{\mathrm{x}}\ F(\mathrm{x}_{\mathcal{S}_1}) + \lambda|\mathcal{S}_1| + H(\mathrm{x}_{\mathcal{S}_1}, 1)$$

Lower bounding

Idea: Convexify a part of the objective function

Node problem

$$p^\nu = \begin{cases} \min_{\mathrm{x},\mathrm{z}} & F(\mathrm{x}) + \lambda \mathbf{1}^{\mathrm{T}}\mathrm{z} + H(\mathrm{x},\mathrm{z}) \\ \text{s.t.} & \mathrm{z}_{\mathcal{S}_0} = 0,\ \mathrm{z}_{\mathcal{S}_1} = 1 \end{cases}$$

$\min_{\mathrm{x},\mathrm{z}} F(\mathrm{x}) + G(\mathrm{x},\mathrm{z})$

Lower bounding

Idea: Convexify a part of the objective function

Node problem

$$p^{\nu} = \begin{cases} \min_{\mathrm{x},\mathrm{z}} & F(\mathrm{x}) + \lambda \mathbf{1}^{\mathrm{T}}\mathrm{z} + H(\mathrm{x},\mathrm{z}) \\ \text{s.t.} & \mathrm{z}_{\mathcal{S}_0} = 0,\ \mathrm{z}_{\mathcal{S}_1} = 1 \end{cases}$$

$\min_{\mathrm{x},\mathrm{z}} F(\mathrm{x}) + G(\mathrm{x},\mathrm{z})$

Bi-conjugacy $G^{\star\star}(\mathrm{x}) \leq G(\mathrm{x},\mathrm{z})$

Lower-bounding problem

$\min_{\mathrm{x}} F(\mathrm{x}) + G^{\star\star}(\mathrm{x})$

Lower bounding

Idea: Convexify a part of the objective function

Node problem

$$p^{\nu} = \begin{cases} \min_{\mathbf{x},\mathbf{z}} & F(\mathbf{x}) + \lambda \mathbf{1}^{\mathrm{T}}\mathbf{z} + H(\mathbf{x},\mathbf{z}) \\ \text{s.t.} & \mathbf{z}_{\mathcal{S}_0} = 0,\ \mathbf{z}_{\mathcal{S}_1} = 1 \end{cases}$$

$\min_{\mathbf{x},\mathbf{z}} F(\mathbf{x}) + G(\mathbf{x},\mathbf{z})$

$\boxed{\text{Bi-conjugacy } G^{\star\star}(\mathbf{x}) \leq G(\mathbf{x},\mathbf{z})}$

Closed-form expression

Lower-bounding problem

$\min_{\mathbf{x}} F(\mathbf{x}) + G^{\star\star}(\mathbf{x})$

Let's sum up !

ℓ_0-penalized problem

$$\min_x \; F(x) + \lambda\|x\|_0$$

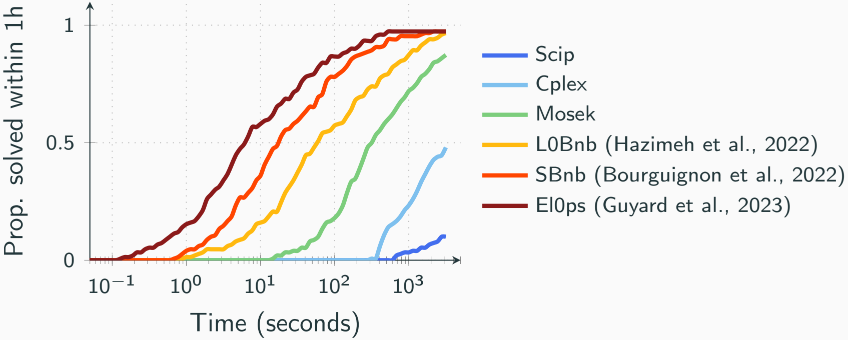
- Linking function $H(x, z)$ to linearize the ℓ_0-norm and fit the MIP formalism
  - Big-M and L2-norm strategies
- Generic solvers
  - Easy solution to implement
  - Unable to exploit sparsity
  - Numerically inefficient
- Specialized Branch-and-Bound
  - Tree exploration
  - Branch by fixing entries in z
  - Compute upper and lower bounds at each node
  - Leverage bi-conjugacy to compute lower bounds

Overview of Numerical Performances

Overview of numerical performances

$$\min_x \; F(x) + \lambda \mathbf{1}^{\mathrm{T}} z + H(x,z)$$

Dataset : Sparse regression
F(·) : Least-squares loss
H(·, ·) : Big-M constraints
λ : Set statistically



Ongoing Research Directions

Contributors and research works

Non-exhaustive list

MIT
D. Bertsimas, R. Mazmuder, ...
MIO tools for ℓ_0-problems

Google Deep Mind
H. Hazimeh, A. Dedieu, ...
MIO-based heuristics and softwares

Lund University
M. Carlsson, C. Olsson...
Quadratic envelope

Frankfurt / Wurzburg Universities
C. Kanzow, A. Tillmann, ...
Optimality conditions

Berkley
A. Atamtürk, A. Gomès, ...
Convex-based acceleration

London Business School
J. Pauphilet, R. Cory-Wright, ...
Healthcare applications

Ponts ParisTech
M. De Lara, P. Chancelier, A. Parmentier, ...
Non-convex analysis for ℓ_0-norm, ML appli.

Centrale Nantes / ENSTA Bretagne
S. Bourguignon, J. Ninin, ...
Branch-and-Bound for ℓ_0-problems

Inria / CentraleSupélec
C. Herzet, C. Elvira, A. Arslan, ...
Generalization, acceleration

IRIT / I3S
E. Soubies, L. Blanc-Féraud, ...
Strong relax. of ℓ_0-norm

Take-home message

- In some cases, solving ℓ_0-norm problems exactly worths-it
- There exists Mixed-Integer Optimization tools to do so
- Structure exploitation is the key to achieve competitive performances
- Active research area

  $\rightarrow$ Theoretical results

  $\rightarrow$ Efficiency, flexibility and accessibility of solution methods

  $\rightarrow$ Software development

  $\rightarrow$ Diffusion to other communities

Question time

🤓

Supplementary Slides

$(\mathcal{S}_0, \mathcal{S}_1)$

Node problem

$$p^{\nu} = \begin{cases} \min & F(\mathrm{x}) + \lambda 1^{\mathrm{T}} \mathrm{z} + H(\mathrm{x}, \mathrm{z}) \\ \text{s.t.} & \mathrm{z}_{\mathcal{S}_0} = 0,\ \mathrm{z}_{\mathcal{S}_1} = 1 \end{cases}$$

Lower bounding

N_k

$(\mathcal{S}_0, \mathcal{S}_1)$

Node problem

$$p^\nu = \begin{cases} \min & F(\mathrm{x}) + \lambda \mathbf{1}^{\mathrm{T}}\mathrm{z} + H(\mathrm{x}, \mathrm{z}) \\ \text{s.t.} & \mathrm{z}_{\mathcal{S}_0} = 0,\ \mathrm{z}_{\mathcal{S}_1} = 1 \end{cases}$$

$\min_{\mathrm{x},\mathrm{z}} P(\mathrm{x}, \mathrm{z})$

Lower bounding

N_k

$(\mathcal{S}_0, \mathcal{S}_1)$

Node problem

$$p^\nu = \begin{cases} \min & F(\mathrm{x}) + \lambda \mathbf{1}^{\mathrm{T}}\mathrm{z} + H(\mathrm{x}, \mathrm{z}) \\ \text{s.t.} & \mathrm{z}_{\mathcal{S}_0} = 0,\ \mathrm{z}_{\mathcal{S}_1} = 1 \end{cases}$$

$\min_{\mathrm{x},\mathrm{z}} P(\mathrm{x}, \mathrm{z})$

$\boxed{\text{Bi-conjugacy } P^{\star\star}(\mathrm{x}, \mathrm{z}) \leq P(\mathrm{x}, \mathrm{z})}$

Lower-bounding problem

$$\tilde{p}^\nu = \min_{\mathrm{x},\mathrm{z}} P^{\star\star}(\mathrm{x}, \mathrm{z})$$

Lower bounding

N_k

$(\mathcal{S}_0, \mathcal{S}_1)$

Node problem

$$p^{\nu} = \begin{cases} \min & F(\mathrm{x}) + \lambda \mathbf{1}^{\mathrm{T}}\mathrm{z} + H(\mathrm{x}, \mathrm{z}) \\ \text{s.t.} & \mathrm{z}_{\mathcal{S}_0} = 0,\ \mathrm{z}_{\mathcal{S}_1} = 1 \end{cases}$$

$\min_{\mathrm{x},\mathrm{z}} P(\mathrm{x}, \mathrm{z})$

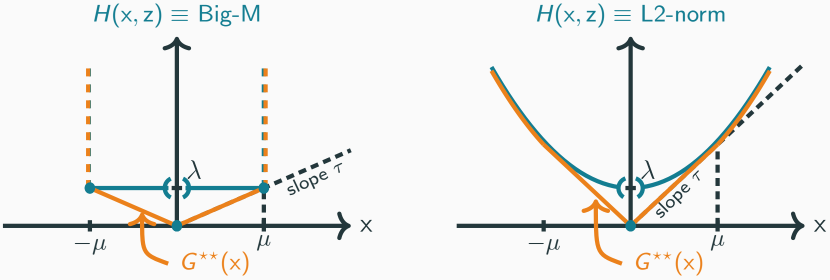
$\boxed{\text{Bi-conjugacy } P^{\star\star}(\mathrm{x}, \mathrm{z}) \leq P(\mathrm{x}, \mathrm{z})}$

Lower-bounding problem

$$\tilde{p}^{\nu} = \min_{\mathrm{x},\mathrm{z}} P^{\star\star}(\mathrm{x}, \mathrm{z})$$

Bi-conjugate computation is also NP-hard

Graphical intuition



Bi-conjugate closed-form

$$G^{\star\star}(x) = \begin{cases} \tau|x| & \text{if } |x| \leq \mu \\ \lambda + H(x, 1) & \text{otherwise} \end{cases}$$

Overview of numerical performances

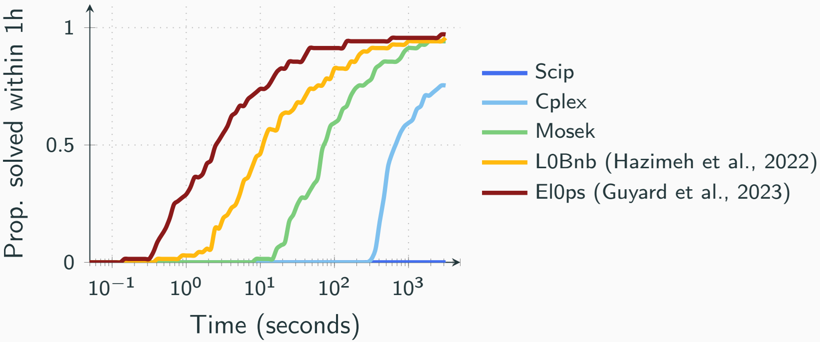
$$\min_x \; F(x) + \lambda 1^T z + H(x, z)$$

Dataset : Sparse regression

F(·) : Least-squares loss

H(·, ·) : L2-norm

λ : Set statistically



Overview of numerical performances

$$\min_{x} \ F(x) + \lambda \mathbf{1}^{\mathrm{T}} z + H(x, z)$$

Dataset : Sparse classification
F(·) : Logistic loss
H(·, ·) : L2-norm
$\boldsymbol{\lambda}$: Set statistically