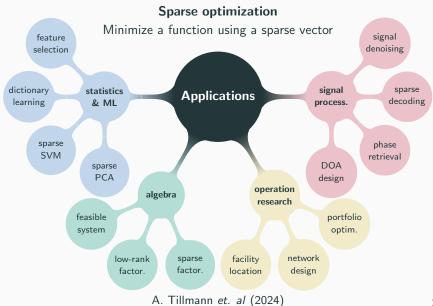
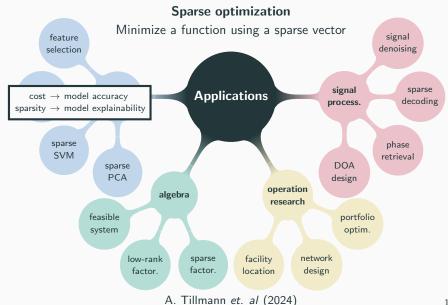
Théo Guyard CIRRELT, Montréal, Canada - March 6th, 2025

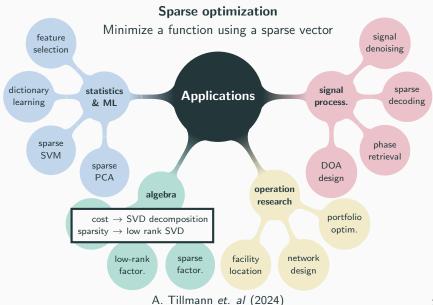
Optimization methods for ℓ_0 -problems

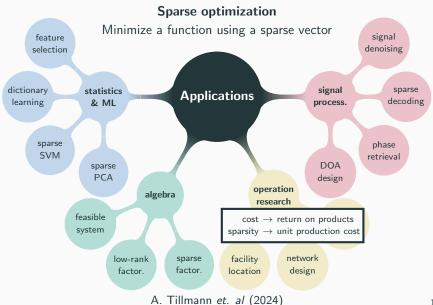
Sparse optimization

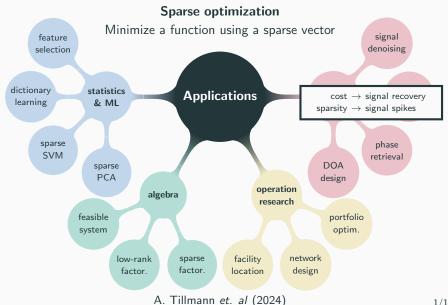
Minimize a function using a sparse vector











Sparse optimization

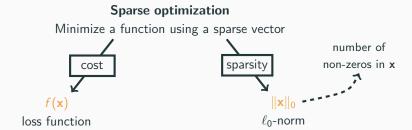
Minimize a function using a sparse vector

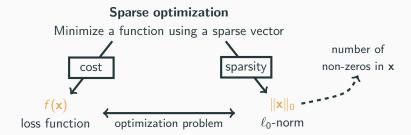
Sparse optimization

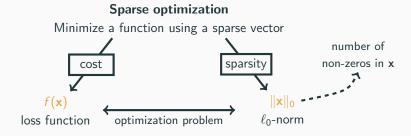
Minimize a function using a sparse vector cost

 $f(\mathbf{x})$

loss function

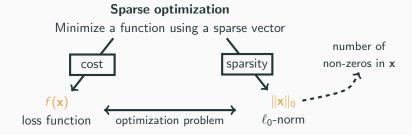






Constrained problem $\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x})$

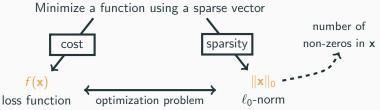
subject to $\|\mathbf{x}\|_0 \leq s$



Constrained problem $\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x})$ subject to $\|\mathbf{x}\|_0 \le s$

$\begin{aligned} & \text{Minimized problem} \\ & \min_{\mathbf{x} \in \mathbf{R}^n} & \|\mathbf{x}\|_0 \\ & \text{subject to} & f(\mathbf{x}) \leq \epsilon \end{aligned}$





Constrained problem

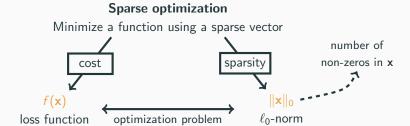
$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x})$$
subject to $\|\mathbf{x}\|_0 \le s$

Minimized problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{x}\|_0$$
 subject to $f(\mathbf{x}) \le \epsilon$

Regularized problem

$$\min_{\mathbf{x}\in\mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0$$



Constrained problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + h(\mathbf{x})$$

subject to $\|\mathbf{x}\|_0 \le s$

Minimized problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} \|\mathbf{x}\|_0 + h(\mathbf{x})$$

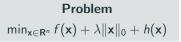
subject to $f(\mathbf{x}) \le \epsilon$

Regularized problem

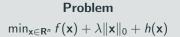
$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

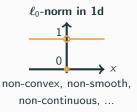
Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



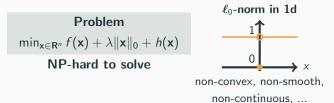




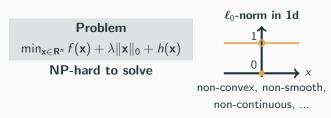


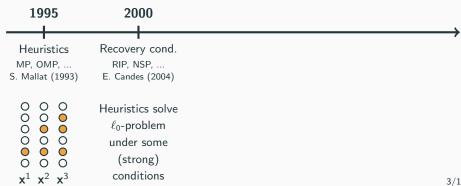
Problem $\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$ NP-hard to solve $0 \longrightarrow x$ non-convex, non-smooth,

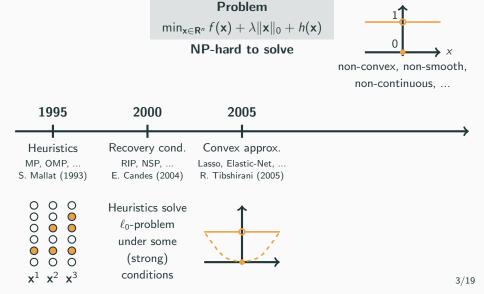
non-continuous, ...



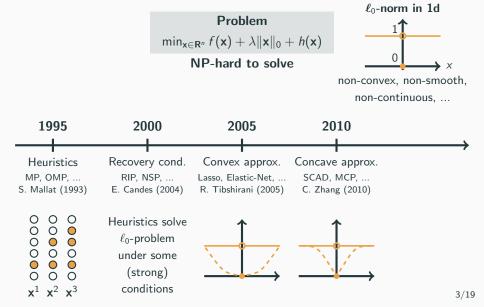


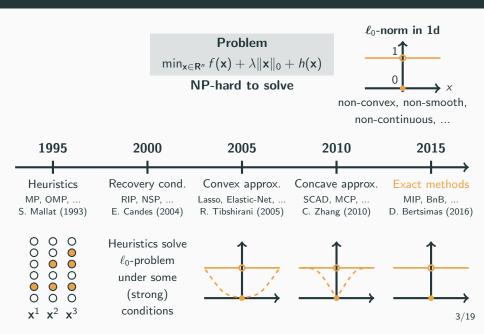


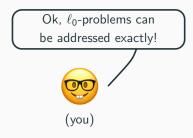


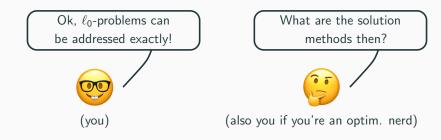


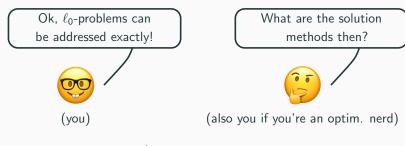
 ℓ_0 -norm in 1d



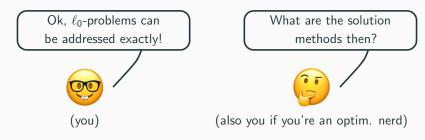








1) MIP-based methods Based on off-the-shelf solvers Poor numerical performances



1) MIP-based methods

Based on off-the-shelf solvers Poor numerical performances

2) BnB-based methods

Tailored solution method
Better numerical performances

Mixed-Integer Programming

Application

ML, Stats, Signal, Operation Research, ...



Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

Application

ML, Stats, Signal, Operation Research, ...



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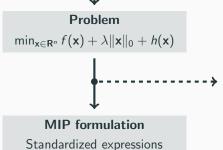


MIP formulation

Standardized expressions



ML, Stats, Signal, Operation Research, ...

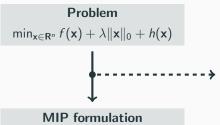


Modelling framework

 $\begin{array}{c} \mathsf{Python} \to \mathsf{cvxpy} \\ \mathsf{Julia} \to \mathsf{JuMP} \\ \mathsf{C}{++} \to \mathsf{CMPL} \\ \mathsf{Matlab} \to \mathsf{YALMIP} \\ & \cdots \end{array}$



ML, Stats, Signal, Operation Research, ...



Standardized expressions

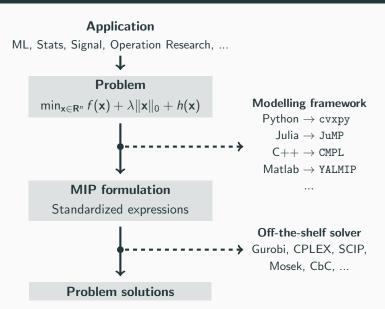
Problem solutions

Modelling framework

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...



MIP – Formulation

Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

MIP formulation

Use standardized expressions linear, quadratic, conic, ...

MIP - Formulation

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MIP formulation

Use standardized expressions linear, quadratic, conic, ...

Linearize the ℓ_0 -norm

We have $\|\mathbf{x}\|_0 = \mathbf{1}^{\mathrm{T}}\mathbf{z}$ whenever $z_i = 0 \iff x_i = 0, \ \forall i$ $z_i = 1 \iff x_i \neq 0, \ \forall i$ for all $\mathbf{x} \in \mathbf{R}^n$ and $\mathbf{z} \in \{0,1\}^n$

MIP - Formulation

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$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



Linearized formulation

$$\begin{cases} \min \ f(\mathbf{x}) + \lambda \mathbf{1}^{\mathrm{T}} \mathbf{z} + h(\mathbf{x}) \\ \text{s.t.} \ z_{i} = 0 \implies x_{i} = 0, \ \forall i \\ \mathbf{x} \in \mathbf{R}^{n}, \ \mathbf{z} \in \{0, 1\}^{n} \end{cases}$$

MIP formulation

Use standardized expressions linear, quadratic, conic, ...

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Avoid logical constraint

$$ilde{h}(\mathbf{x},\mathbf{z}) = egin{cases} h(\mathbf{x}) & ext{if } z_i = x_i = 0 ext{ or } z_i = 1, orall i \ +\infty & ext{otherwise} \end{cases}$$

MIP - Formulation

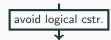
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MIP formulation

$$\begin{cases} \min \ f(\mathbf{x}) + \lambda \mathbf{1}^{\mathrm{T}} \mathbf{z} + \tilde{h}(\mathbf{x}, \mathbf{z}) \\ \text{s.t. } \mathbf{x} \in \mathbf{R}^{n}, \ \mathbf{z} \in \{0, 1\}^{n} \end{cases}$$

MIP formulation

Use standardized expressions linear, quadratic, conic, ...

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Two existing strategies to design $\tilde{h}(x,z)$

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Big-M strategy

$$h(\mathbf{x}) = \sum_{i=1}^{n} \operatorname{Cstr}(|x_{i}| \leq M)$$
with $M > 0$

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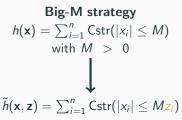
Big-M strategy
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$$\downarrow$$

$$\tilde{h}(\mathbf{x}, \mathbf{z}) = \sum_{i=1}^{n} \operatorname{Cstr}(|x_i| \leq M_{Z_i})$$

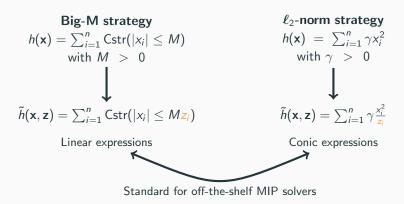
$$\begin{array}{l} \ell_2\text{-norm strategy} \\ h(\mathbf{x}) \ = \ \sum_{i=1}^n \gamma x_i^2 \\ \text{with} \ \gamma \ > \ 0 \end{array}$$

$$\tilde{h}(\mathbf{x}, \mathbf{z}) = \begin{cases} h(\mathbf{x}) & \text{if } z_i = x_i = 0 \text{ or } z_i = 1, \forall i \\ +\infty & \text{otherwise} \end{cases}$$





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MIP – Let's sum up

Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

Pipeline

- 1) Introduce binary variable $\mathbf{z} \in \{0,1\}^n$
- 2) Linearize ℓ_0 -norm as $\|\mathbf{x}\|_0 = \mathbf{1}^{\mathrm{T}}\mathbf{z}$
- 3) Transform h(x) into $\tilde{h}(x,z)$
- 4) Use generic MIP solvers

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Pros

- ✓ Rich MIP literature
- ✓ Black-box solvers
- ✓ Straightforward pipeline

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- 4) Use generic MIP solvers

Pros

- ✓ Rich MIP literature
- ✓ Black-box solvers
- ✓ Straightforward pipeline

Cons

- X Mostly commercial solvers
- **X** Only for $h = \text{big-M}/\ell_2$ -norm
- X Performance issues

Branch-and-Bound Algorithms

Application

ML, Stats, Signal, Operation Research, ...



Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

Application

ML, Stats, Signal, Operation Research, ...



Problem

 $\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$



Implement BnB solver

Specialized mechanisms

Application

ML, Stats, Signal, Operation Research, ...



Problem

 $\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$

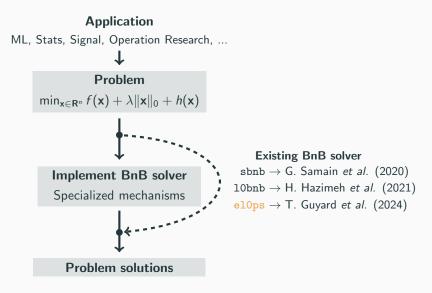


Implement BnB solver

Specialized mechanisms

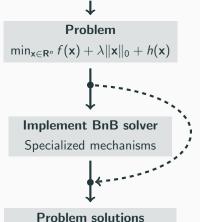


Problem solutions





ML, Stats, Signal, Operation Research, ...

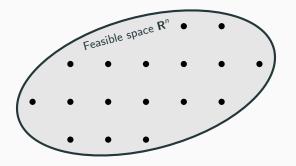


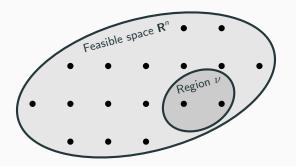
Existing BnB solver

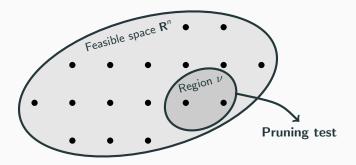
 ${\tt sbnb} \to {\tt G.}$ Samain et al. (2020) 10bnb $\to {\tt H.}$ Hazimeh et al. (2021) el0ps $\to {\tt T.}$ Guyard et al. (2024)

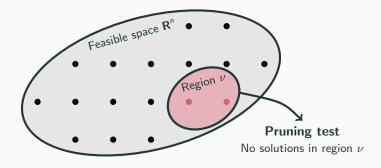
Why using elops?
Is is free, fast and flexible!

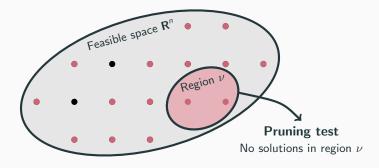




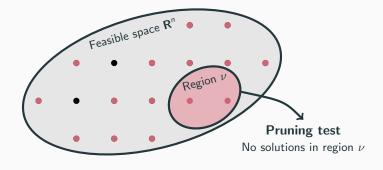








Explore regions in the feasible space and prune those that cannot contain any optimal solution.



Branching step – Region design and exploration **Bounding step** – Pruning test evaluation

Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

Observation

Solutions are expected to be sparse

Problem

 $\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$

Observation

Solutions are expected to be sparse

Method

Drive the sparsity of the optimization variable

Problem
$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

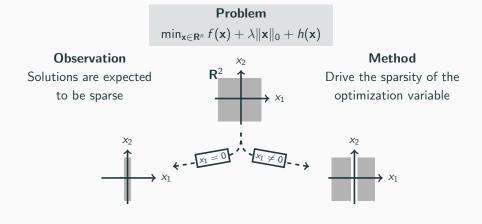
Observation

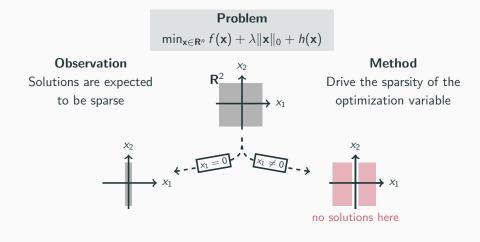
Solutions are expected to be sparse

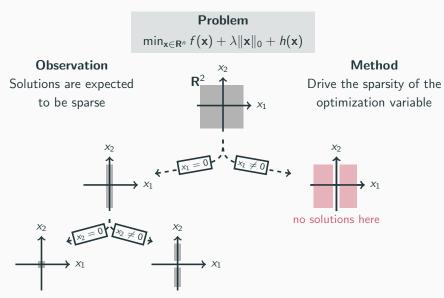


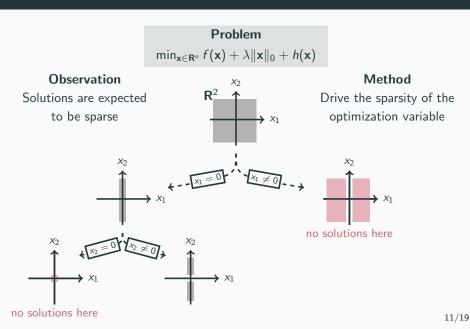
Method

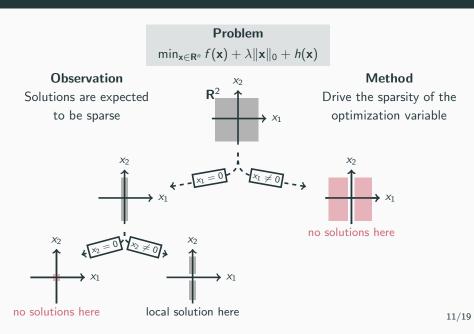
Drive the sparsity of the optimization variable

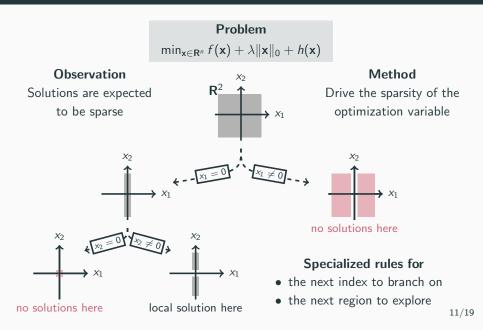












BnB – **Bounding** step



Does region $\boldsymbol{\nu}$ contains optimal solutions ?



Does region $\boldsymbol{\nu}$ contains optimal solutions ?

Problem

$$p^{\star} = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



Does region ν contains optimal solutions ?

Problem

$$p^{\star} = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \boldsymbol{\nu}} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_{0} + h(\mathbf{x})$$



Does region ν contains optimal solutions ?

Problem

$$p^{\star} = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



Restriction to region ν

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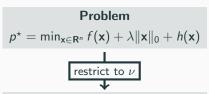


Pruning test

$$p^{\nu} > p^{\star}$$



Does region ν contains optimal solutions ?



Restriction to region ν

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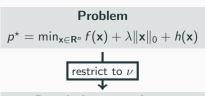
Pruning test

$$p^{\nu} > p^{\star}$$

 \rightarrow prune ν



Does region ν contains optimal solutions ?



Restriction to region ν

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Pruning test

$$p_{
m lb}^{
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Does region ν contains optimal solutions ?

Problem

$$p^{\star} = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$



Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \nu} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



Pruning test

$$p^{
u}_{
m lb} > p^{\star}_{
m ub}$$

 \longrightarrow prune ν

Easy task

Compute an upper bound on p^*



Does region ν contains optimal solutions ?

Problem

$$p^* = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \nu} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



Pruning test

$$p_{
m lb}^{
u}>p_{
m ub}^{\star}$$



Easy task

Compute an upper bound on p^*

Construct and evaluate a feasible vector in each region explored to refine p_{ub}^{\star}



Does region ν contains optimal solutions ?

Problem

$$p^* = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$



Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \boldsymbol{\nu}} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_{0} + h(\mathbf{x})$$



Pruning test

$$p_{
m lb}^{
u}>p_{
m ub}^{\star}$$



Easy task

Compute an upper bound on p^*

Construct and evaluate a feasible vector in each region explored to refine p_{ub}^*

Main challenge

Compute a lower bound on p^{ν}



Does region ν contains optimal solutions ?

Problem

$$p^{\star} = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \nu} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



Pruning test

$$p_{
m lb}^{
u}>p_{
m ub}^{\star}$$

 \rightarrow prune ν

Easy task

Compute an upper bound on p^*

Construct and evaluate a feasible vector in each region explored to refine p_{ub}^{\star}

Main challenge

Compute a lower bound on p^{ν}

Construct and solve a relaxation

BnB – Building relaxations

Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \nu} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

seek tight/tractable lower bound on p^{ν}

BnB – Building relaxations

Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \nu} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$

reformulation

Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \mathbf{g}^{\nu}(\mathbf{x})$$

seek tight/tractable lower bound on p^{ν}

with g^{ν} proper and closed

BnB – Building relaxations

Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \nu} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_{0} + h(\mathbf{x})$$

reformulation

Restriction to region ν

$$p^{\nu} = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \mathbf{g}^{\nu}(\mathbf{x})$$

$$g_{\mathsf{lb}}^{\nu} \leq g^{\nu}, g_{\mathsf{lb}}^{\nu} \mathsf{convex}$$

Relaxation for region ν

$$p_{\mathsf{lb}}^{\nu} = \mathsf{min}_{\mathsf{x} \in \mathsf{R}^n} f(\mathsf{x}) + g_{\mathsf{lb}}^{\nu}(\mathsf{x})$$

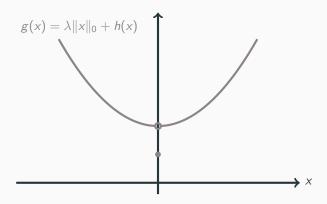
seek tight/tractable lower bound on p^{ν}

with g^{ν} proper and closed

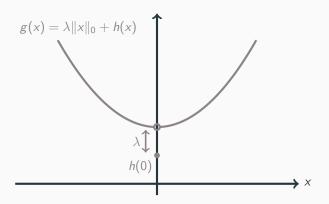
set $g_{\mathrm{lb}}^{\,
u}$ set as the convex envelope of $g^{\,
u}$

Convex envelope of $g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$ with $\mathbf{x} \in \mathbf{R}^n$

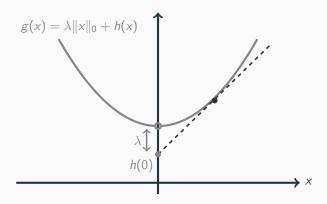
Convex envelope of $g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$ with $\mathbf{x} \in \mathbf{R}^n$ h separable and coercive



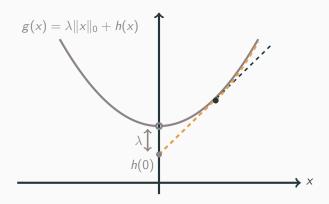
Convex envelope of $g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$ with $\mathbf{x} \in \mathbf{R}^n$ h separable and coercive



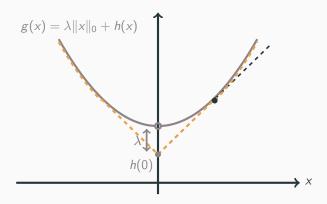
Convex envelope of $g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$ with $\mathbf{x} \in \mathbf{R}^n$ h separable and coercive



Convex envelope of $g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$ with $\mathbf{x} \in \mathbf{R}^n$ h separable and coercive



Convex envelope of $g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$ with $\mathbf{x} \in \mathbf{R}^n$ h separable and coercive



Solve time

region processing time \times number of regions processed

Solve time

region processing time \times number of regions processed

Relaxation for region ν

$$\rho_{\mathsf{lb}}^{\nu} = \mathsf{min}_{\mathsf{x} \in \mathsf{R}^n} \, f(\mathsf{x}) + g_{\mathsf{lb}}^{\nu}(\mathsf{x})$$

Solve time

region processing time \times number of regions processed

Relaxation for region ν

$$p_{\mathsf{lb}}^{\nu} = \mathsf{min}_{\mathsf{x} \in \mathsf{R}^n} f(\mathsf{x}) + g_{\mathsf{lb}}^{\nu}(\mathsf{x})$$

 $\textit{g}^{\nu}_{\text{lb}}$ is proper, closed, convex, separable, and non-smooth at x=0

Solve time

region processing time \times number of regions processed

Relaxation for region ν

$$p_{\mathsf{lb}}^{\nu} = \mathsf{min}_{\mathsf{x} \in \mathsf{R}^n} f(\mathsf{x}) + g_{\mathsf{lb}}^{\nu}(\mathsf{x})$$

 $g_{\mathrm{lb}}^{
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This is a convex sparse optimization problem

Solve time

Relaxation for region ν

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 $g_{
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ightarrow first-order methods proximal gradient, coordinate descent, ... ightarrow acceleration strategies working set, screening tests, ...

Solve time

 $\frac{\text{region processing time}}{\checkmark} \times \underline{\text{number of regions processed}}$

Relaxation for region ν

$$p_{\mathsf{lb}}^{\nu} = \mathsf{min}_{\mathsf{x} \in \mathsf{R}^n} f(\mathsf{x}) + g_{\mathsf{lb}}^{\nu}(\mathsf{x})$$

 g_{lb}^{ν} is proper, closed, convex, separable, and non-smooth at x=0

This is a **convex** sparse optimization problem

→ first-order methods
 proximal gradient, coordinate descent, ...
 → acceleration strategies
 working set, screening tests, ...

Simultaneous pruning

Solve time

region processing time \times number of regions processed

Relaxation for region ν

$$p_{\mathsf{lb}}^{\nu} = \mathsf{min}_{\mathsf{x} \in \mathsf{R}^n} f(\mathsf{x}) + g_{\mathsf{lb}}^{\nu}(\mathsf{x})$$

 $g^{
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→ first-order methods
 proximal gradient, coordinate descent, ...
 → acceleration strategies
 working set, screening tests, ...

Simultaneous pruning



processing region ...

Solve time

 $\frac{\text{region processing time}}{\checkmark} \times \frac{\text{number of regions processed}}{\checkmark}$

Relaxation for region ν

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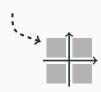
This is a convex sparse optimization problem

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Simultaneous pruning



processing region ...



Solve time

 $\frac{\text{region processing time}}{\checkmark} \times \frac{\text{number of regions processed}}{\checkmark}$

Relaxation for region ν

$$p_{\mathsf{lb}}^{\nu} = \mathsf{min}_{\mathsf{x} \in \mathsf{R}^n} \, f(\mathsf{x}) + g_{\mathsf{lb}}^{\nu}(\mathsf{x})$$

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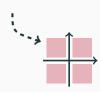
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processing region ...



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This is a convex sparse optimization problem

→ first-order methods

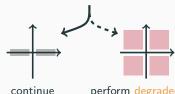
proximal gradient, coordinate descent, ...

 \rightarrow acceleration strategies working set, screening tests, ...

Simultaneous pruning



processing region ...



continue processing

Solve time

region processing time \times number of regions processed

Relaxation for region ν

$$p_{\mathsf{lb}}^{\nu} = \min_{\mathbf{x} \in \mathsf{R}^n} f(\mathbf{x}) + g_{\mathsf{lb}}^{\nu}(\mathbf{x})$$

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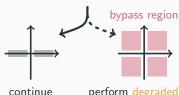
This is a convex sparse optimization problem

- \rightarrow first-order methods proximal gradient, coordinate descent, ...
 - \rightarrow acceleration strategies working set, screening tests, ...

Simultaneous pruning



processing region ...



continue processing

BnB – Let's sum up

Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

Pipeline

- 1a) Implement a BnB solver
- **1b)** Use an existing BnB solver
 - 2) Solve the problem

BnB – Let's sum up

Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

Pipeline

- 1a) Implement a BnB solver
- **1b)** Use an existing BnB solver
 - **2)** Solve the problem

Pros

- ✓ Numerical efficiency
- ✓ Open-source softwares
- ✓ Any h separable and coercive

BnB – Let's sum up

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- **1a)** Implement a BnB solver
- **1b)** Use an existing BnB solver
 - 2) Solve the problem

Pros

- ✓ Numerical efficiency
- ✓ Open-source softwares
- ✓ Any h separable and coercive

Cons

X Less standard pipeline

Numerical Illustration

Numerics – Feature Selection Problem

Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

MIP solvers: → cplex → mosek BnB solvers: → 10bnb → el0ps

Numerics – Feature Selection Problem

Problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

Instance 1

- $f(x) = \frac{1}{2} ||y Ax||_2^2$
- $h(\mathbf{x}) = \frac{\gamma}{2} \|\mathbf{x}\|_2^2 + \mathsf{Cstr}(\|\mathbf{x}\|_{\infty} \leq M)$
- riboflavin dataset with $\mathbf{A} \in \mathbf{R}^{71 \times 4088}$

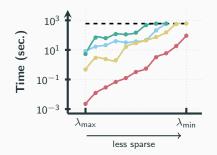
Numerics – Feature Selection Problem

Problem
$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$

MIP solvers: → cplex → mosek BnB solvers: → 10bnb → el0ps

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Numerics – Feature Selection Problem

Problem

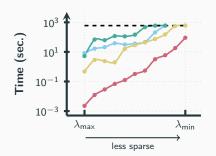
$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

MIP solvers: → cplex → mosek

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- $f(\mathbf{x}) = \frac{1}{2} ||\mathbf{y} \mathbf{A}\mathbf{x}||_2^2$
- $h(\mathbf{x}) = \frac{\gamma}{2} \|\mathbf{x}\|_2^2 + \mathsf{Cstr}(\|\mathbf{x}\|_{\infty} \leq M)$
- riboflavin dataset with $\mathbf{A} \in \mathbf{R}^{71 \times 4088}$



Instance 2

- $f(x) = \mathbf{1}^{\mathrm{T}} \log(1 + \exp(-y \odot Ax))$
- $h(\mathbf{x}) = \gamma \|\mathbf{x}\|_1 + \mathsf{Cstr}(\|\mathbf{x}\|_{\infty} \leq M)$
- ullet leukemia dataset with ${f A} \in {f R}^{38 imes 7129}$

Numerics – Feature Selection Problem

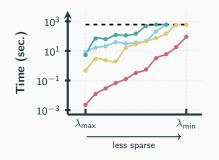
Problem $\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$

MIP solvers: → cplex → mosek

BnB solvers: → 10bnb → el0ps

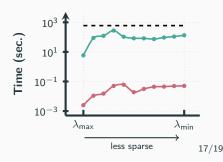
Instance 1

- $f(\mathbf{x}) = \frac{1}{2} ||\mathbf{y} \mathbf{A}\mathbf{x}||_2^2$
- $h(\mathbf{x}) = \frac{\gamma}{2} \|\mathbf{x}\|_2^2 + \mathsf{Cstr}(\|\mathbf{x}\|_{\infty} \leq M)$
- riboflavin dataset with $\mathbf{A} \in \mathbf{R}^{71 \times 4088}$



Instance 2

- $f(x) = 1^T \log(1 + \exp(-y \odot Ax))$
- $h(\mathbf{x}) = \gamma \|\mathbf{x}\|_1 + \mathsf{Cstr}(\|\mathbf{x}\|_{\infty} \leq M)$
- leukemia dataset with $\mathbf{A} \in \mathbf{R}^{38 \times 7129}$



Conclusion

on-exhaustive list

Non-exhaustive list



Convex-based acceleration

Non-exhaustive list



MIT D. Bertsimas, R. Mazmuder, ... Optimization tools for ℓ_0 -problems **Lund University** Google Deep Mind M. Carlsson, C. Olsson... H. Hazimeh, A. Dedieu, ... Relaxation design MIP-hased heuristics Frankfurt / Wurzburg Universities C. Kanzow, A. Tillmann, ... Optimality conditions London Business School Berkley A. Atamtürk, A. Gomès, ... J. Pauphilet, R. Cory-Wright, ... Convex-based acceleration Healthcare applications

18/19

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Take-home messages

- Although NP-hard, ℓ_0 -problems are of practical interest
- There exists methods to tackle them exactly
 - MIP-based formulation and off-the-shelf solvers
 - BnB-based specialized algorithms
 - Structure-exploitation is key for numerical efficiency
- It's an active research area
 - Theoretical and methodological developments still missing
 - Need to reach the application world

Question time!

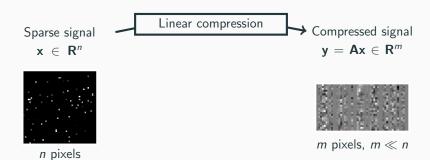


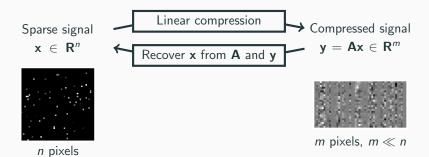
Sparse signal

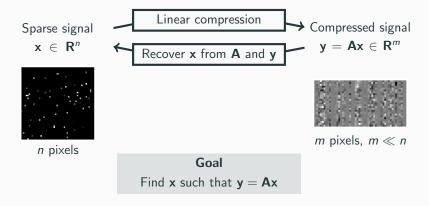
 $x \in R^n$

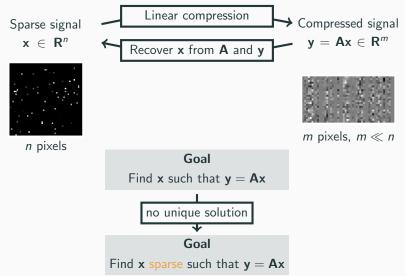


n pixels









	Feature 1	Feature 2		Feature n	Target
Sample 1	a _{1,1}	a _{1,2}		$a_{1,n}$	<i>y</i> ₁
Sample 2	a _{2,1}			$a_{2,n}$	
Sample 3	<i>a</i> _{3,1}	$A \in R^{mx}$	< n	<i>a</i> _{3,n}	$y \in R^m$
Sample m	$a_{m,1}$			$a_{m,n}$	Ут

	Feature 1	Feature 2		Feature n	Target
Sample 1	a _{1,1}			$a_{1,n}$	
Sample 2	a _{2,1}			$a_{2,n}$	
Sample 3	a _{3,1}	$A \in R^{m}$	×n	a _{3,n}	$y \in R^m$
Sample m	$a_{m,1}$			$a_{m,n}$	Ут

Features
$$\mathbf{A} \in \mathbf{R}^{m \times n} \longleftrightarrow \mathbf{A} \in \mathbf{R}^m \longleftrightarrow \mathbf{A} \times \mathbf{A} \times \mathbf{A}$$
 Target $\mathbf{y} = \phi(\mathbf{A}\mathbf{x})$

	Feature 1	Feature 2		Feature n	Target
Sample 1	$a_{1,1}$			$a_{1,n}$	
Sample 2	a _{2,1}			$a_{2,n}$	
Sample 3	a _{3,1}	$A \in R^{m}$	≺ n	a _{3,n}	$y \in R^m$
Sample m	$a_{m,1}$			$a_{m,n}$	Ут

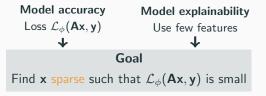
Features
$$\mathbf{A} \in \mathbf{R}^{m \times n} \longleftrightarrow \mathbf{Weights} \ \mathbf{x} \in \mathbf{R}^n \Longrightarrow \mathbf{Target} \ \mathbf{y} = \phi(\mathbf{A}\mathbf{x})$$

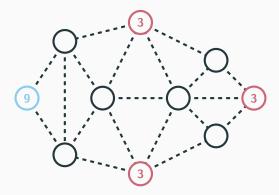
Model accuracy Loss $\mathcal{L}_{\phi}(\mathbf{A}\mathbf{x},\mathbf{y})$

Model explainability
Use few features

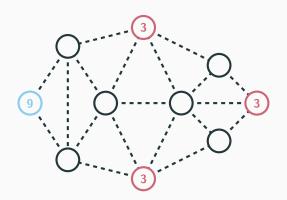
	Feature 1	Feature 2		Feature n	Target
Sample 1	a _{1,1}			$a_{1,n}$	
Sample 2	a _{2,1}			a _{2,n}	
Sample 3	a _{3,1}	$A \in R^{m}$	×n	a _{3,n}	$y \in R^m$
Sample m	$a_{m,1}$	$a_{m,2}$		$a_{m,n}$	Ут

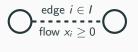
Features
$$\mathbf{A} \in \mathbf{R}^{m \times n} \longleftrightarrow \mathbf{A} \in \mathbf{R}^m \longleftrightarrow \mathbf{A} \times \mathbf{A} = \mathbf{A} \times \mathbf{A}$$



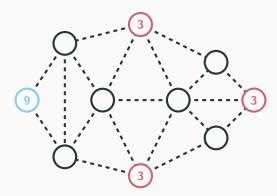


Which edges to build to transport products from source to sink nodes?





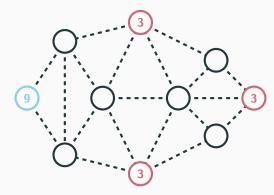
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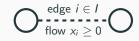
Which edges to build to transport products from source to sink nodes?



construct edge $i \in I$ if $x_i > 0$ pay construction cost c



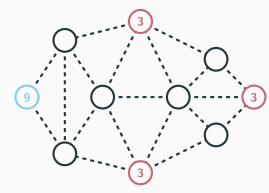
Which edges to build to transport products from source to sink nodes?



construct edge $i \in I$ if $x_i > 0$ pay construction cost c

Question

How to construct the least number of edges to satisfy transportation needs?



Which edges to build to transport products from source to sink nodes?



construct edge $i \in I$ if $x_i > 0$ pay construction cost c

Question

How to construct the least number of edges to satisfy transportation needs?



Balancing solution quality and problem hardness

Riboflavin dataset - P. Bühlmann et al. (2014)

Colony	AADK	AAPA	ABFA	ABH	 ZUR	B2 prod.
#1	8.49	8.11	8.32	10.28	 7.42	-6.64 -5.43
#2	7.29	6.39	11.32	9.42	 6.99	-5.43
#71	 6.85	 8.27	7.98	8.04	 6.65	-7.58

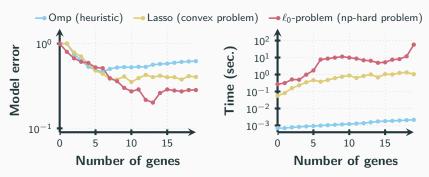
4,088 genes

Balancing solution quality and problem hardness

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						 -7.58

4,088 genes



Sparse regression Find x sparse such that $y \simeq Ax$

Sparse regression

Find x sparse such that $y \simeq Ax$

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathsf{Cstr}(-M \le \mathbf{x} \le M)$

Sparse regression

Find x sparse such that $y \simeq Ax$

Optimization problem

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- $h(\mathbf{x}) = \mathsf{Cstr}(-M \le \mathbf{x} \le M)$



MIP formulation

$$\begin{cases} \min \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \mathbf{1}^{\mathrm{T}}\mathbf{z} \\ \text{s.t.} & -M\mathbf{z} \leq \mathbf{x} \leq M\mathbf{z} \\ \mathbf{x} \in \mathbf{R}^n, \ \mathbf{z} \in \{0,1\}^n \end{cases}$$

Sparse regression

Find x sparse such that $y \simeq Ax$



$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathsf{Cstr}(-M \le \mathbf{x} \le M)$

1

MIP formulation

$$\begin{cases} \min \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \mathbf{1}^{\mathrm{T}}\mathbf{z} \\ \text{s.t.} \quad -M\mathbf{z} \leq \mathbf{x} \leq M\mathbf{z} \\ \mathbf{x} \in \mathbf{R}^n, \ \mathbf{z} \in \{0, 1\}^n \end{cases}$$

Sparse regression

Find x sparse such that $y \simeq Ax$



Optimization problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathsf{Cstr}(-M \le \mathbf{x} \le M)$



MIP formulation

$$\begin{cases} \min \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_{2}^{2} + \lambda \mathbf{1}^{\mathrm{T}}\mathbf{z} \\ \text{s.t.} \quad -M\mathbf{z} \leq \mathbf{x} \leq M\mathbf{z} \\ \mathbf{x} \in \mathbf{R}^{n}, \ \mathbf{z} \in \{0, 1\}^{n} \end{cases}$$

\$ pip install cvxpy

import cvxpy as cp

Generate sparse regression data
A, y = make_regression()

Sparse regression

Find x sparse such that $y \simeq Ax$

Optimization problem

$$\min_{\mathbf{x}\in\mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
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MIP formulation

$$\begin{cases} \min \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_{2}^{2} + \lambda \mathbf{1}^{\mathrm{T}}\mathbf{z} \\ \text{s.t.} \quad -M\mathbf{z} \leq \mathbf{x} \leq M\mathbf{z} \\ \mathbf{x} \in \mathbf{R}^{n}, \ \mathbf{z} \in \{0, 1\}^{n} \end{cases}$$

```
import cvxpy as cp

# Generate sparse regression data
A, y = make_regression()

# Define variables
n = A.shape[1]
x = cp.Variable(n)
z = cp.Variable(n, boolean=True)
```

Sparse regression

Find x sparse such that $y \simeq Ax$

Optimization problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
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MIP formulation

$$\begin{cases} \min \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \mathbf{1}^{\mathrm{T}} \mathbf{z} \\ \text{s.t.} \quad -M \mathbf{z} \leq \mathbf{x} \leq M \mathbf{z} \\ \mathbf{x} \in \mathbf{R}^n, \ \mathbf{z} \in \{0, 1\}^n \end{cases}$$

```
import cvxpy as cp
# Generate sparse regression data
A, y = make_regression()
# Define variables
n = A.shape[1]
x = cp.Variable(n)
z = cp. Variable(n, boolean=True)
# Define objective and constraints
obi = cp.Minimize(
    cp.sum_squares(A @ x - y) +
    0.01 * cp.sum(z)
cst = [-5.0 * z \le x, x \le 5.0 * z]
```

Sparse regression

Find x sparse such that $y \simeq Ax$

Optimization problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \operatorname{Cstr}(-M \le \mathbf{x} \le M)$

MIP formulation

$$\begin{cases} \min \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \mathbf{1}^{\mathrm{T}}\mathbf{z} \\ \text{s.t.} \quad -M\mathbf{z} \leq \mathbf{x} \leq M\mathbf{z} \\ \mathbf{x} \in \mathbf{R}^n, \ \mathbf{z} \in \{0, 1\}^n \end{cases}$$

```
import cvxpy as cp
# Generate sparse regression data
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# Define objective and constraints
obi = cp.Minimize(
    cp.sum_squares(A @ x - y) +
    0.01 * cp.sum(z)
cst = [-5.0 * z \le x, x \le 5.0 * z]
# Solve the problem using Gurobi
problem = cp.Problem(obj, cst)
problem.solve(solver=cp.GUROBI)
```

 $\label{eq:sparse regression} \begin{aligned} \text{Find } \mathbf{x} \text{ sparse such} \\ \text{that } \mathbf{y} \ \simeq \ \mathbf{A}\mathbf{x} \end{aligned}$

Sparse regression

Find x sparse such

that y \simeq Ax



$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathsf{Cstr}(-M \le \mathbf{x} \le M)$

\$ pip install el0ps

Sparse regression

Find \mathbf{x} sparse such

that y \simeq Ax



$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathsf{Cstr}(-M \le \mathbf{x} \le M)$

\$ pip install el0ps

Sparse regression Find x sparse such that y ≃ Ax ↓

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathsf{Cstr}(-M \le \mathbf{x} \le M)$

```
from el0ps.datafits import Leastsquares
from el0ps.penalties import Bigm
from el0ps.solvers import BnbSolver

# Generate sparse regression data
A, y = make_regression()
```

\$ pip install el0ps

Sparse regression Find x sparse such that y \simeq Ax

$$\min_{\mathbf{x}\in\mathbf{R}^n}f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

- $\bullet \ f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathsf{Cstr}(-M \le \mathbf{x} \le M)$

```
from elOps.datafits import Leastsquares
from elOps.penalties import Bigm
from elOps.solvers import BnbSolver

# Generate sparse regression data
A, y = make_regression()

# Instantiate the loss and penalty
f = Leastsquares(A, y)
h = Bigm(M=5.0)
```

\$ pip install el0ps

Sparse regressionFind **x** sparse such

that
$$\mathbf{y} \simeq \mathbf{A}\mathbf{x}$$



$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda ||\mathbf{x}||_0 + h(\mathbf{x})$$

- $f(\mathbf{x}) = \frac{1}{2} \|\mathbf{y} \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathsf{Cstr}(-M \le \mathbf{x} \le M)$

```
from elops.datafits import Leastsquares
from elops.penalties import Bigm
from elops.solvers import BnbSolver

# Generate sparse regression data
A, y = make_regression()

# Instantiate the loss and penalty
f = Leastsquares(A, y)
h = Bigm(M=5.0)

# Solve the problem with elops' solver
solver = BnbSolver()
solver.solve(f, h, lmbd=0.01)
```