

Branch-and-Bound Algorithms for ℓ_0 -Regularized Problems

Théo Guyard

Inria and Insa Rennes

PhD defense - November 27th, 2024

Problem

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

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1) Loss $f(\mathbf{Ax})$

Models the quantity
to minimize in the
application at hand

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2) ℓ_0 -norm $\|\mathbf{x}\|_0$

Counts non-zeros in
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Models the quantity to minimize in the **application** at hand

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Counts non-zeros in its input to promote **sparse** solutions

3) Penalty $h(\mathbf{x})$

Linked to the **application** or artificially introduced to enable **solution methods**

ℓ_0 -regularized problems

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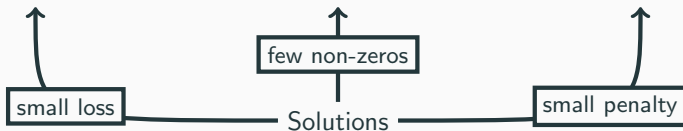
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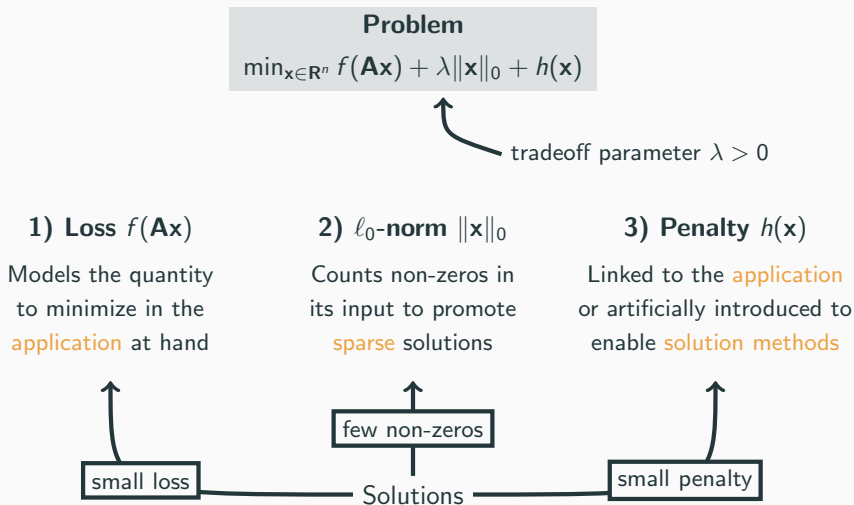
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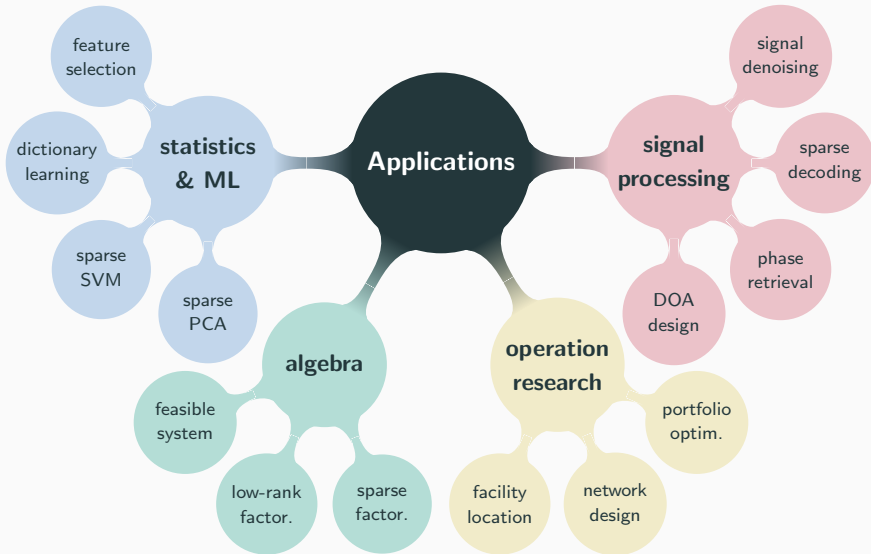
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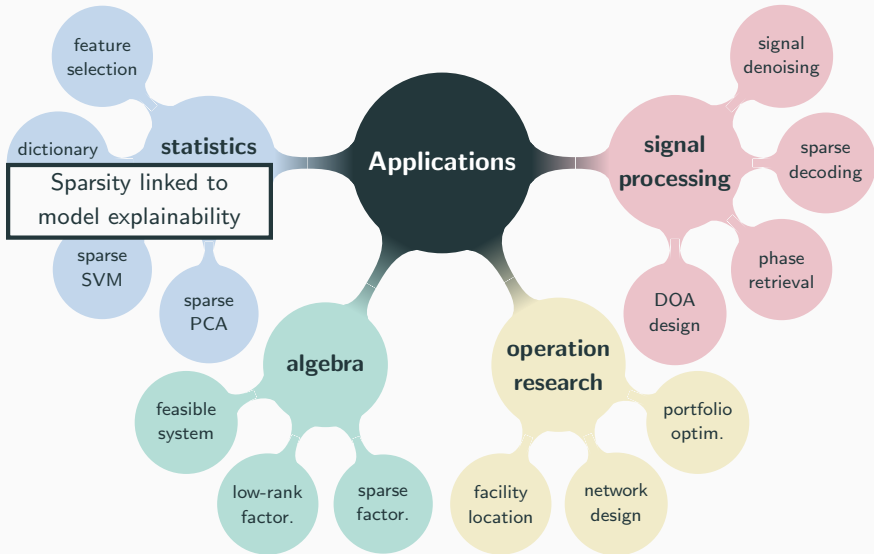
ℓ_0 -regularized problems



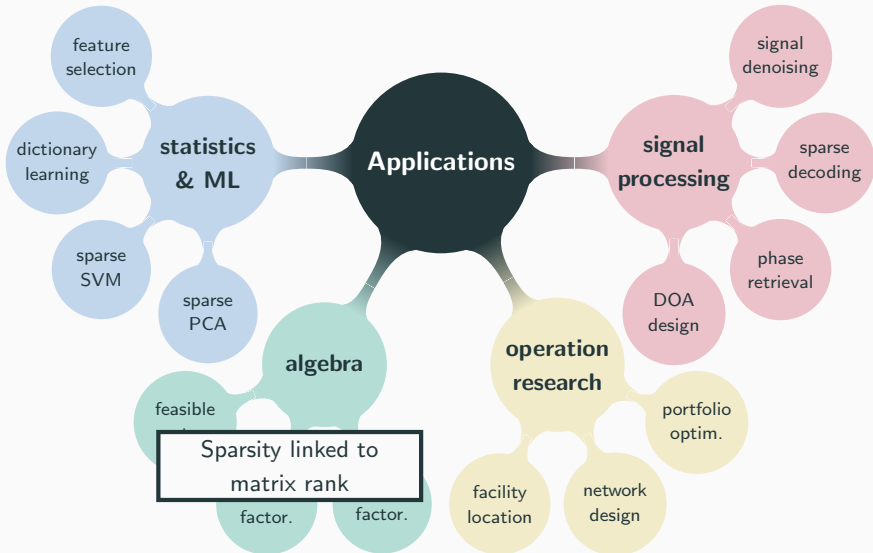
One problem to rule them all



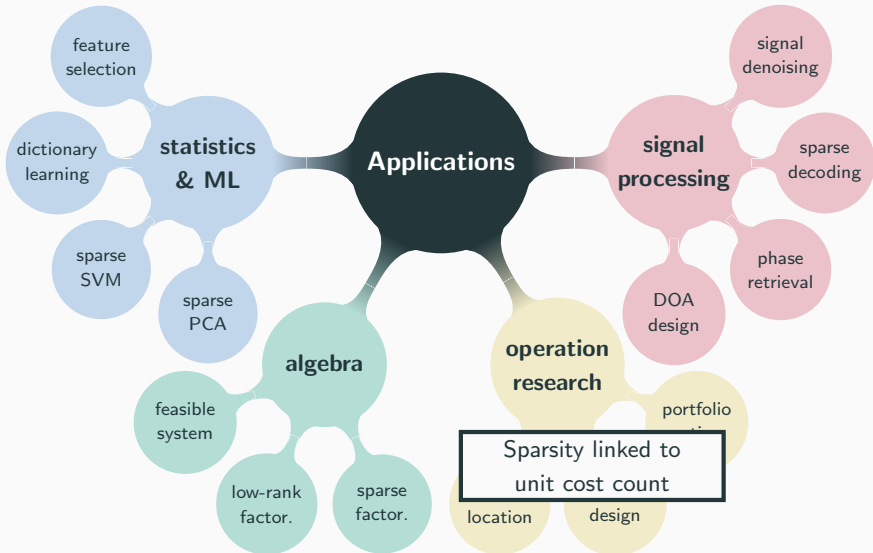
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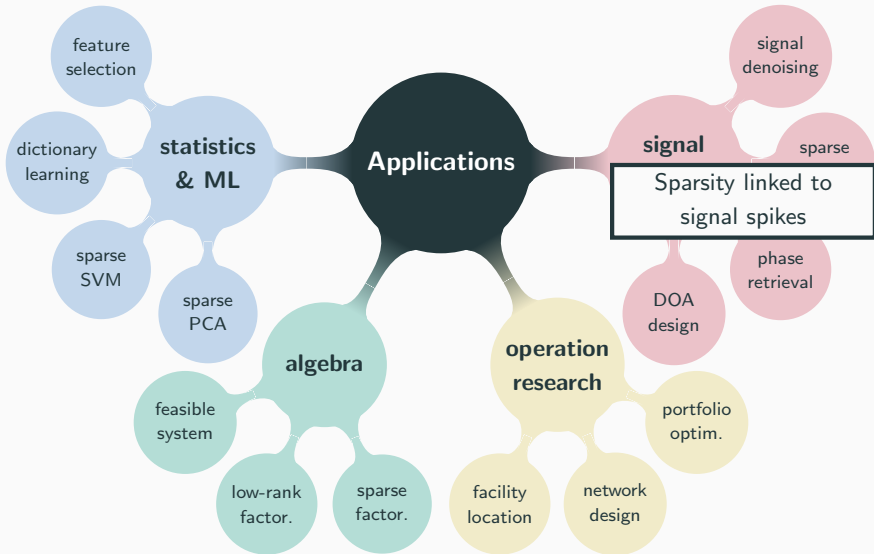
One problem to rule them all



One problem to rule them all



One problem to rule them all



Problem

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

Question

How to design **generic** and **efficient** solution methods ?

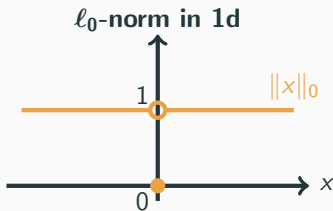
Solution methods

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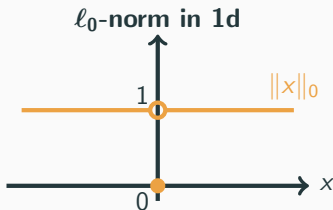
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How to design **generic** and **efficient** solution methods ?



Properties

- non-convex
- non-smooth
- non-continuous
- ...

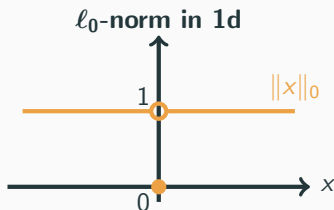
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**Can be tackled using
generic MIP solvers**

D. Bertsimas *et. al* (2016)

Problem

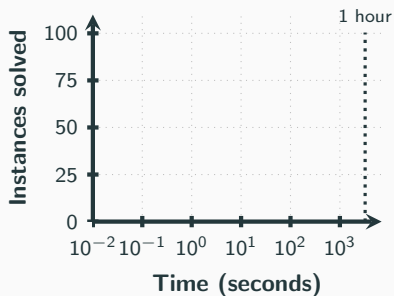
$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

$\mathbf{A} \in \mathbb{R}^{100 \times 300}$ / f : Quadratic / h : Bound constraint

Problem

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

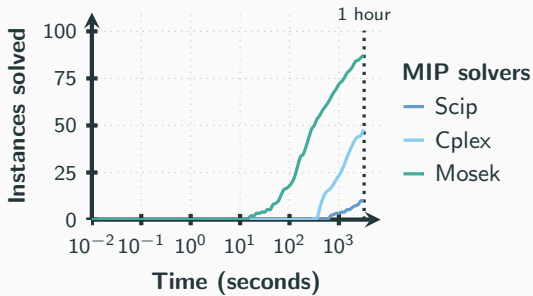
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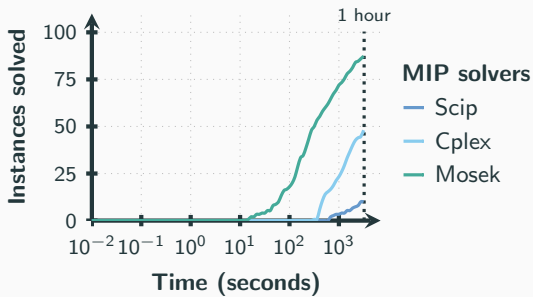
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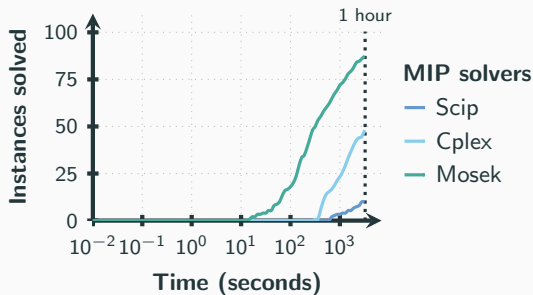


Can we do better ?

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Can we do better ?



BnB solvers

Specialized for the
problem at hand

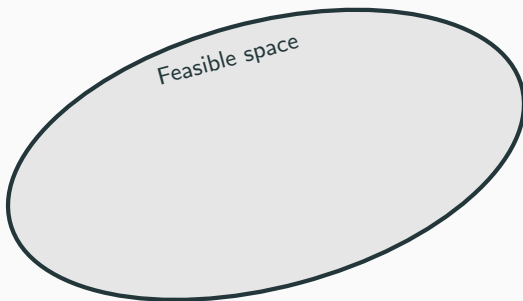
Branch-and-Bound Algorithms

BnB – Algorithmic principle

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

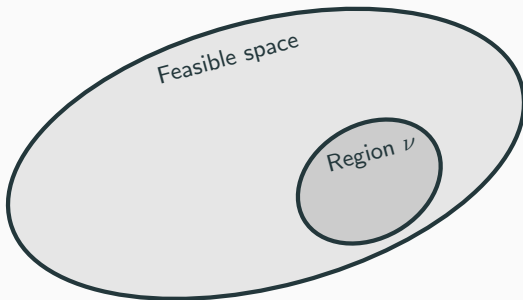
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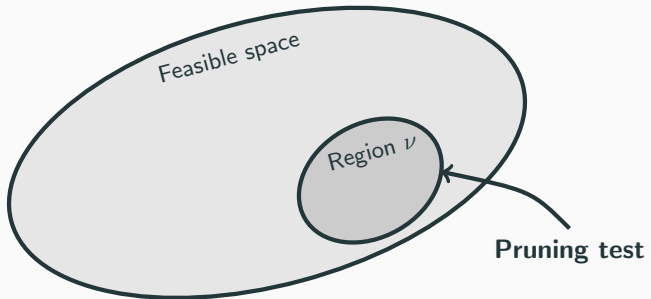
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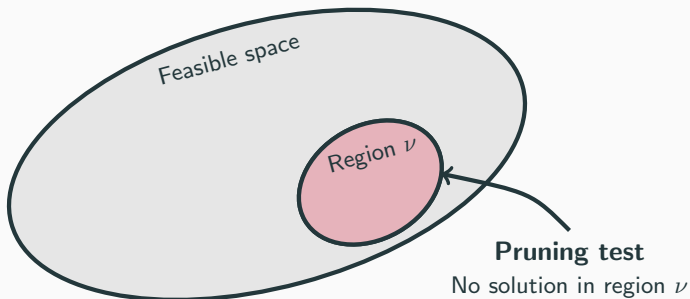
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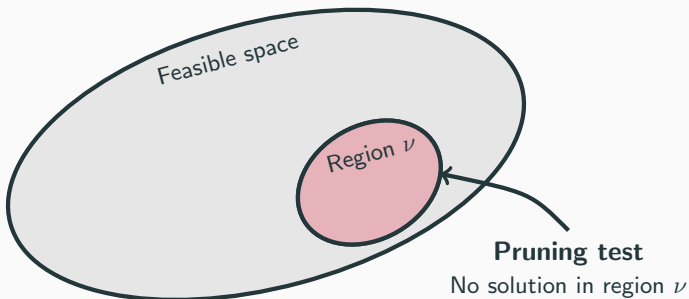
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Explore **regions** in the feasible space and **prune** those that cannot contain any optimal solution.



BnB – Algorithmic principle

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Branching – Region management

Bounding – Pruning test evaluation

BnB – How to construct regions in the feasible space ?

Problem

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

BnB – How to construct regions in the feasible space ?

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

Observation

Solutions expected
to be sparse

BnB – How to construct regions in the feasible space ?

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Method

Drive the sparsity of the
optimization variable

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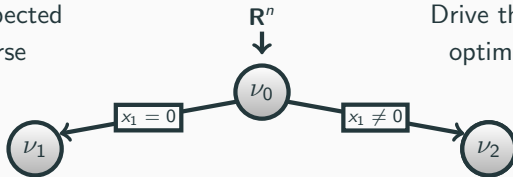
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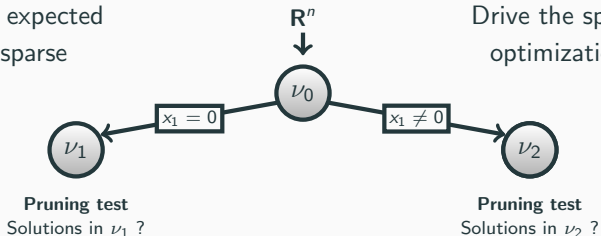
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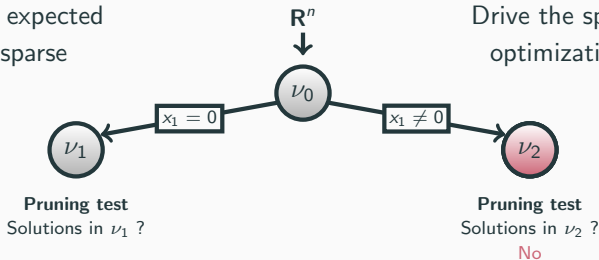
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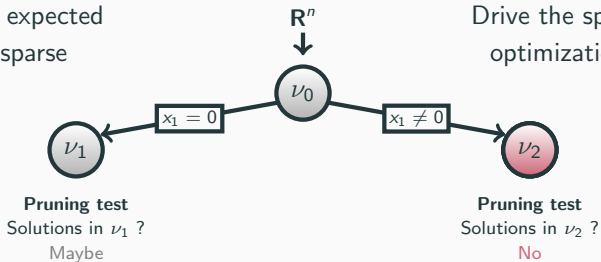
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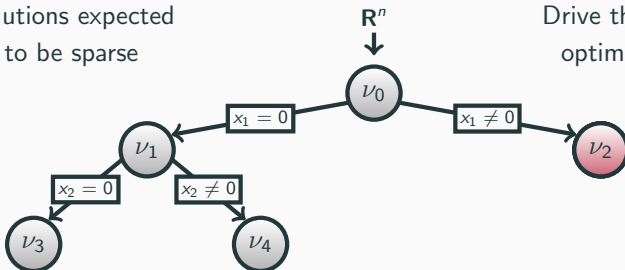
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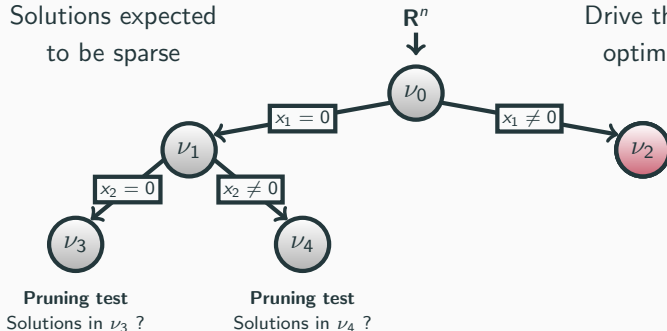
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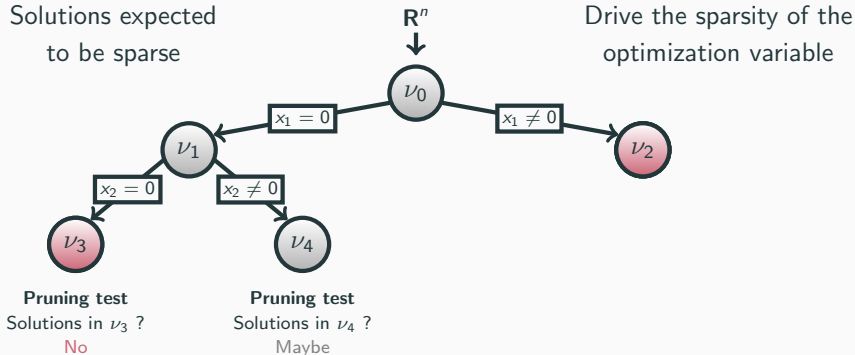
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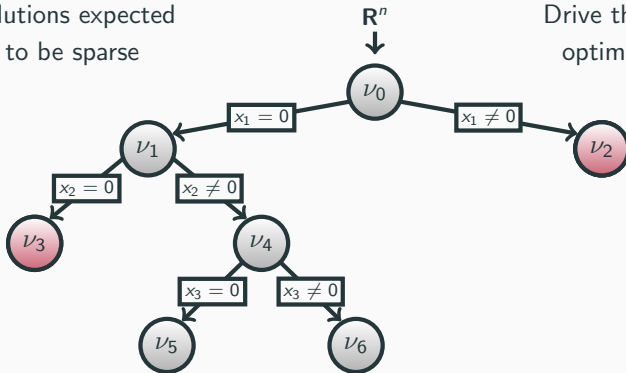
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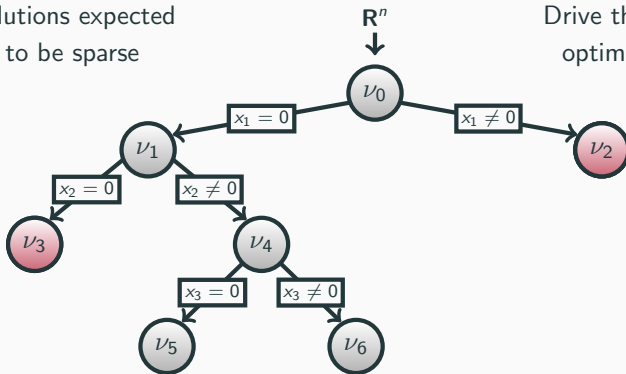
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Observation

Solutions expected
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Method

Drive the sparsity of the
optimization variable



Pruning test
Solutions in ν_5 ?

Pruning test
Solutions in ν_6 ?

BnB – How to construct regions in the feasible space ?

Problem

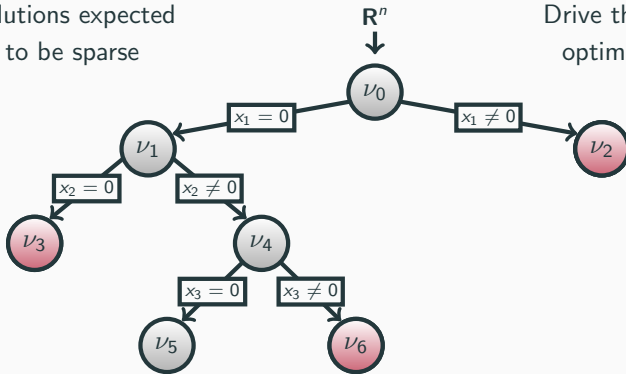
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Observation

Solutions expected
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Method

Drive the sparsity of the
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Pruning test
Solutions in ν_5 ?
Maybe

Pruning test
Solutions in ν_6 ?
No

BnB – How to construct regions in the feasible space ?

Problem

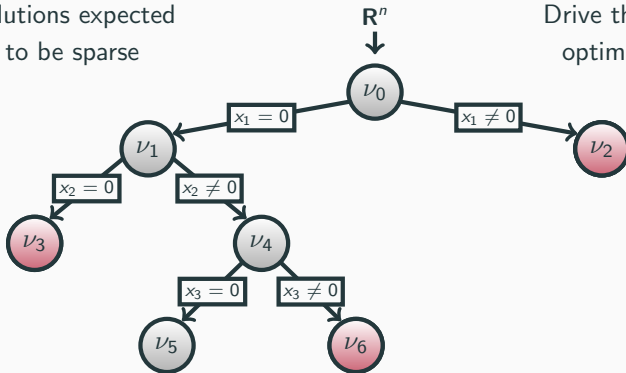
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Method

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Recover
solution

BnB – How to construct regions in the feasible space ?

Problem

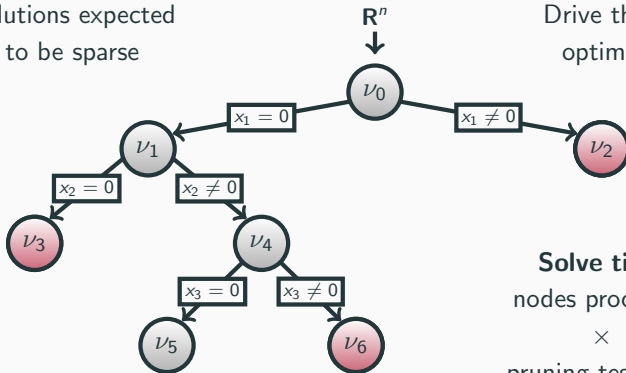
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Observation

Solutions expected
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Method

Drive the sparsity of the
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Recover
solution

Solve time
nodes processed
×
pruning test time

BnB – How to evaluate a pruning test ?



Pruning test

Solutions in region ν ?

BnB – How to evaluate a pruning test ?



Pruning test

Solutions in region ν ?

Problem

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

BnB – How to evaluate a pruning test ?



Pruning test

Solutions in region ν ?

Problem

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

restrict to ν

Restriction to region ν

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

BnB – How to evaluate a pruning test ?



Pruning test

Solutions in region ν ?

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Restriction to region ν

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

compare

Pruning test

$$p^\nu > p^*$$

BnB – How to evaluate a pruning test ?



Pruning test

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Pruning test

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→ prune ν

BnB – How to evaluate a pruning test ?



Pruning test

Solutions in region ν ?

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compare

Pruning test

$$p_{\text{lb}}^\nu > p_{\text{ub}}^*$$

→ prune ν

BnB – How to evaluate a pruning test ?



Pruning test

Solutions in region ν ?

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Pruning test

$$p_{\text{lb}}^\nu > p_{\text{ub}}^*$$

→ prune ν

Easy task

Compute an upper bound on p^*

BnB – How to evaluate a pruning test ?



Pruning test

Solutions in region ν ?

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compare

Pruning test

$$p_{lb}^\nu > p_{ub}^*$$

→ prune ν

Easy task

Compute an upper bound on p^*

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

BnB – How to evaluate a pruning test ?



Pruning test

Solutions in region ν ?

Problem

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Restriction to region ν

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compare

Pruning test

$$p_{\text{lb}}^\nu > p_{\text{ub}}^*$$

→ prune ν

Easy task

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Construct and evaluate
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Main challenge

Compute a lower bound on p^ν

BnB – Standard lower bounding strategy

Restriction to region ν

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

BnB – Standard lower bounding strategy

Restriction to region ν

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

Requirement 1 – Tight lower bound on p^ν

Requirement 2 – Tractable lower bound on p^ν

BnB – Standard lower bounding strategy

Restriction to region ν

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Requirement 1 – Tight lower bound on p^ν

Requirement 2 – Tractable lower bound on p^ν



Standard strategy

Construct and solve a relaxation

BnB – Standard lower bounding strategy

Restriction to region ν

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

Requirement 1 – Tight lower bound on p^ν

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Standard strategy

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BnB – Standard lower bounding strategy

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Requirement 1 – Tight lower bound on p^ν

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Standard strategy

Construct and solve a relaxation

Relaxation for region ν

$$p_{\text{lb}}^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{lb}}(\mathbf{x})$$

BnB – Standard lower bounding strategy

Restriction to region ν

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Requirement 1 – Tight lower bound on p^ν

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Standard strategy

Construct and solve a relaxation

Relaxation for region ν

$$p_{\text{lb}}^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{lb}}(\mathbf{x})$$

$$g_{\text{lb}} \leq g$$

g_{lb} convex

BnB – Standard lower bounding strategy

Restriction to region ν

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Standard strategy

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Relaxation for region ν

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$$g_{\text{lb}} \leq g$$

g_{lb} convex

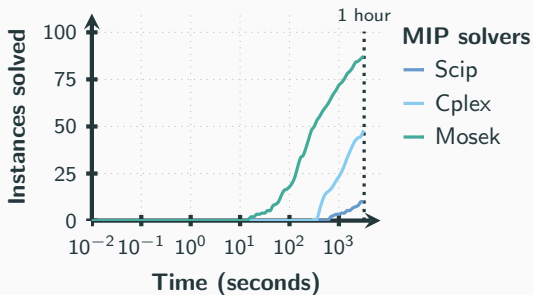
Lower bound

$$p_{\text{lb}}^\nu \leq p^\nu$$

Problem

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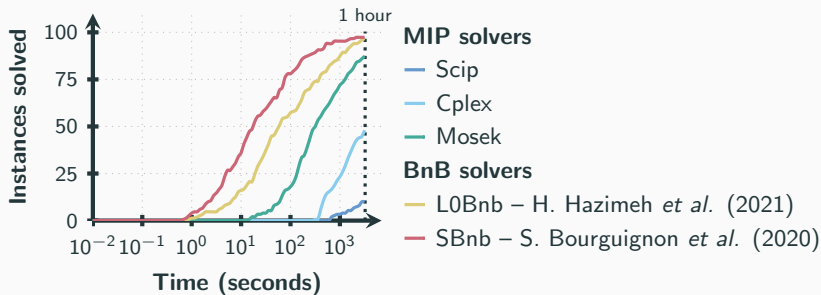
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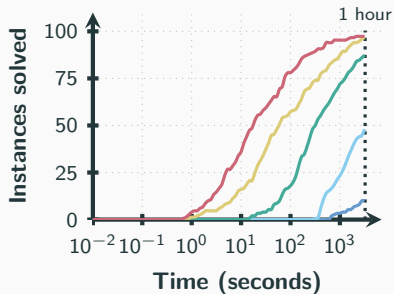
$\mathbf{A} \in \mathbb{R}^{100 \times 300}$ / f : Quadratic / h : Bound constraint



Problem

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MIP solvers

- Scip
- Cplex
- Mosek

BnB solvers

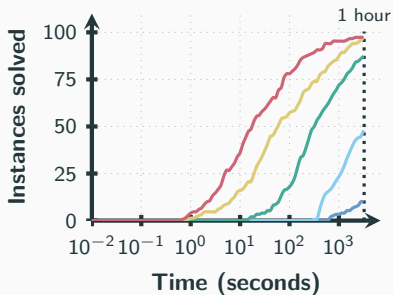
- LOBnb – H. Hazimeh *et al.* (2021)
- SBnb – S. Bourguignon *et al.* (2020)

Observation

Better performance
with BnB solvers

Problem

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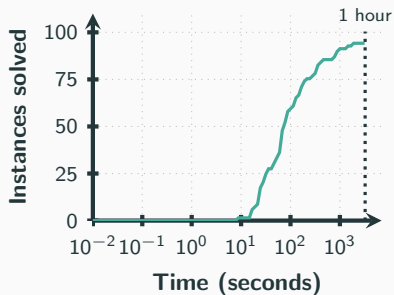
Observation

Better performance
with BnB solvers
... but they are
instance-specific

Problem

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

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MIP solvers

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BnB solvers

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Let's recap

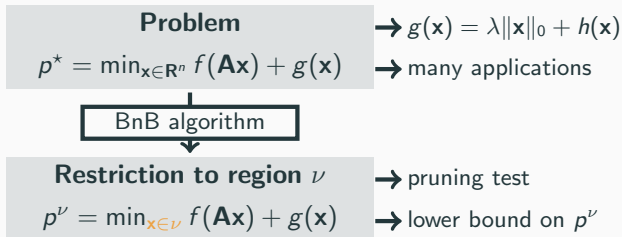
Problem

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

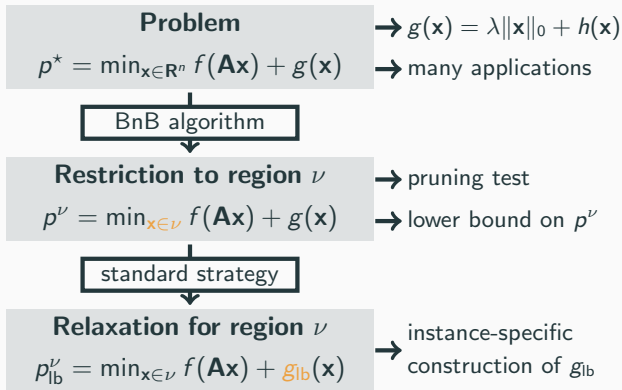
$$\rightarrow g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

\rightarrow many applications

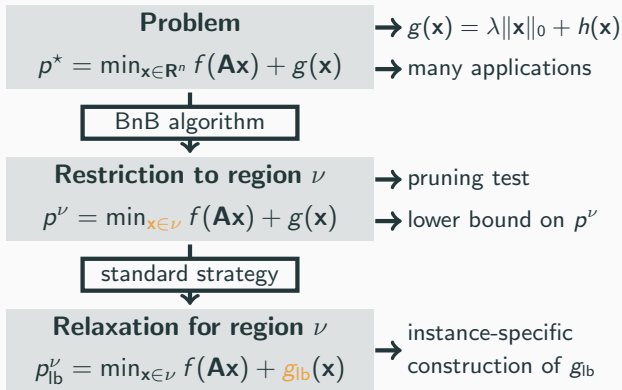
Let's recap



Let's recap



Let's recap



Axis 1

How to construct
relaxations generically ?

Manuscript – Chap. 3

→ Journal paper (202x)

Axis 1 – How to construct relaxations generically ?

Axis 1 – Generic relaxation construction

Restriction to region ν

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

$$g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

lower bound on p^ν

Axis 1 – Generic relaxation construction

Restriction to region ν

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

$$g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

lower bound on p^ν

standard strategy

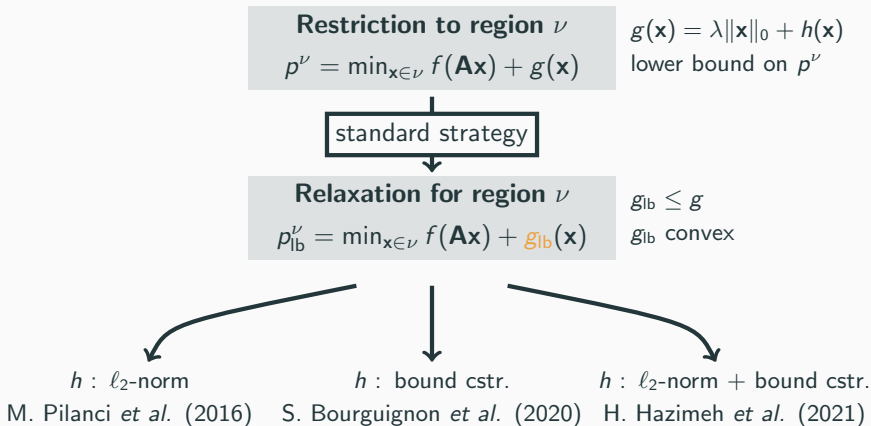
Relaxation for region ν

$$p_{\text{lb}}^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{lb}}(\mathbf{x})$$

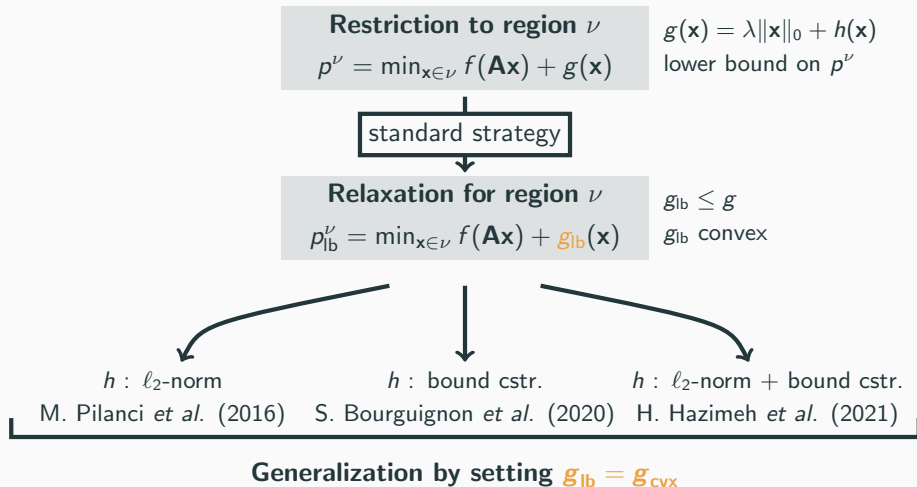
$$g_{\text{lb}} \leq g$$

g_{lb} convex

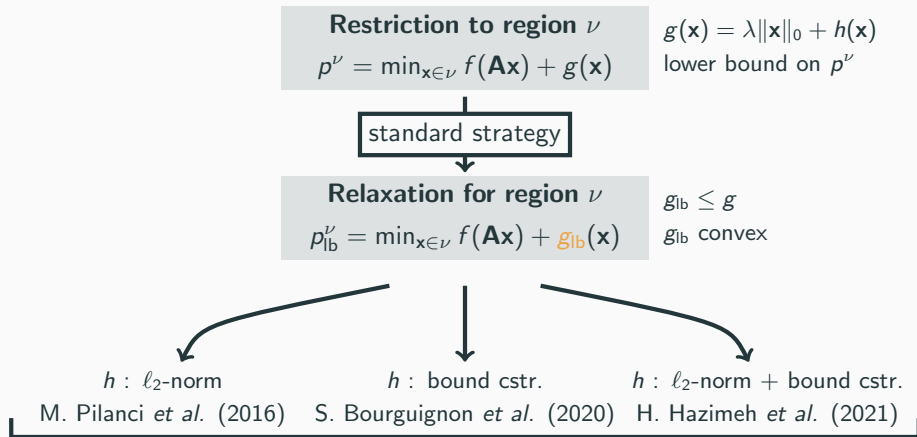
Axis 1 – Generic relaxation construction



Axis 1 – Generic relaxation construction



Axis 1 – Generic relaxation construction



Generalization by setting $g_{\text{lb}} = g_{\text{cvx}}$

→ h proper, closed, convex

→ h separable, even, supercoercive, $h \geq h(\mathbf{0}) = 0$

Axis 1 – Convex envelope characterization

Spotlight result

The convex envelope of $g(\mathbf{x}) = \lambda\|\mathbf{x}\|_0 + h(\mathbf{x})$ admits a closed-form expression.

Axis 1 – Convex envelope characterization

Spotlight result

The convex envelope of $g(\mathbf{x}) = \lambda\|\mathbf{x}\|_0 + h(\mathbf{x})$ admits a closed-form expression.

Theorem (1d version) – Let $g(x) = \lambda\|x\|_0 + h(x)$, one has

$$g_{\text{cvx}}(x) = \begin{cases} \tau|x| & \text{if } |x| \leq \mu \\ h(x) + \lambda & \text{otherwise} \end{cases}$$

where (τ, μ) are some “easy-to-compute” quantities.

Axis 1 – Convex envelope characterization

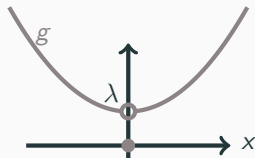
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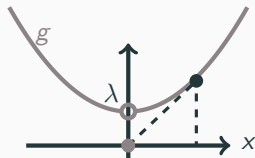
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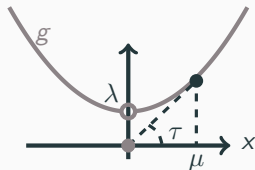
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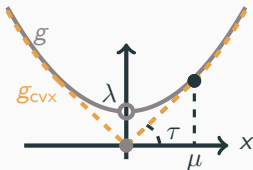
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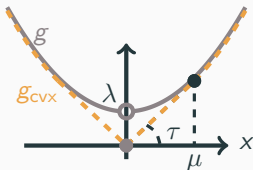
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Generic relaxation construction

Characterize $g_{\text{lb}} = g_{\text{cvx}}$

Encompasses prior contributions

Axis 1 – Convex envelope characterization

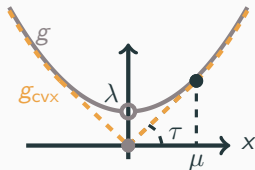
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Generic relaxation construction

Characterize $g_{\text{lb}} = g_{\text{cvx}}$

Encompasses prior contributions



Practical relaxation construction

Closed-form for ∂g_{cvx} and $\text{prox}_{g_{\text{cvx}}}$

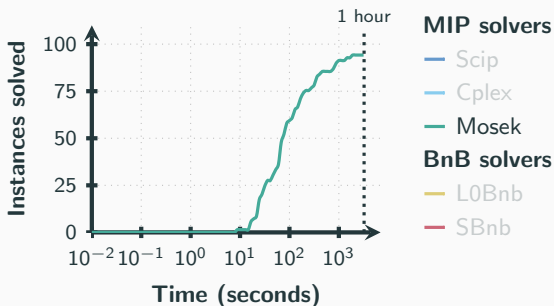
Enables standard solution methods

Axis 1 – Numerics

Problem

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

$\mathbf{A} \in \mathbb{R}^{100 \times 300}$ / f : Logistic / h : Bound cstr. + ℓ_1 -norm

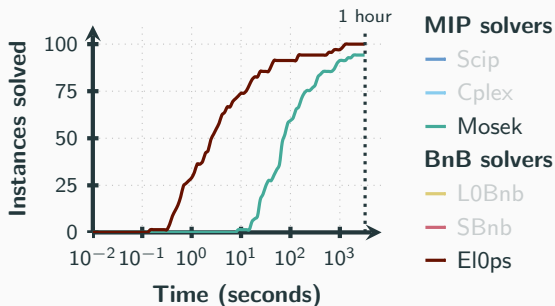


Axis 1 – Numerics

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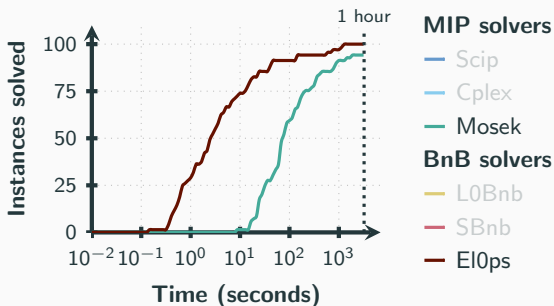


Axis 1 – Numerics

Problem

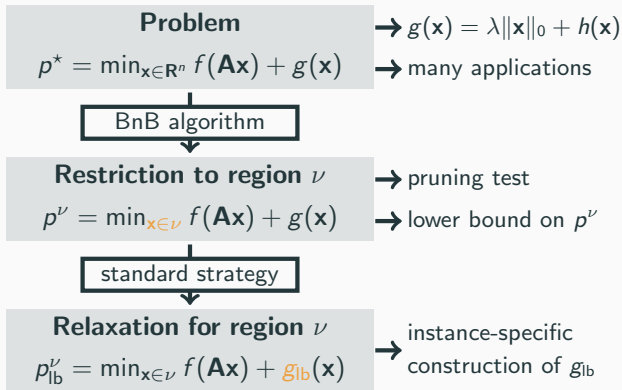
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El0ps is a **generic**
BnB solver with
state-of-the-art
performance

Let's recap

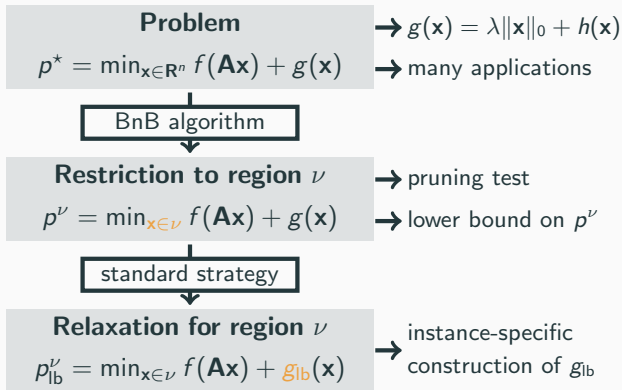


Axis 1

How to construct
relaxations generically ?

- 1) Set $g_{\text{lb}} = g_{\text{cvx}}$
- 2) Closed-form expression
- 3) Generalize BnB method

Let's recap



Axis 1

How to construct relaxations generically ?

- 1) Set $g_{\text{lb}} = g_{\text{cvx}}$
- 2) Closed-form expression
- 3) Generalize BnB method

Axis 2

How to solve relaxations efficiently ?

Manuscript – Chap. 6
→ ICASSP (2022)
→ Journal paper (202x)

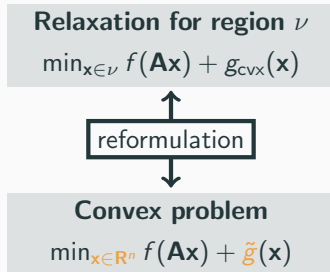
Axis 2 – How to solve relaxations efficiently ?

Axis 2 – Convex optimization

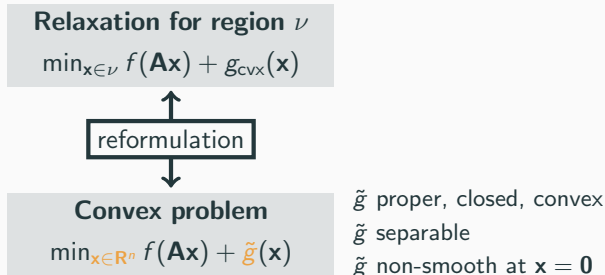
Relaxation for region ν

$$\min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{cvx}}(\mathbf{x})$$

Axis 2 – Convex optimization



Axis 2 – Convex optimization



Axis 2 – Convex optimization

Relaxation for region ν

$$\min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{cvx}}(\mathbf{x})$$

remind g_{cvx} acts as an ℓ_1 -norm near $\mathbf{x} = \mathbf{0}$

reformulation

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

\tilde{g} proper, closed, convex
 \tilde{g} separable
 \tilde{g} non-smooth at $\mathbf{x} = \mathbf{0}$

Axis 2 – Convex optimization

Applications beyond
the BnB scope



Relaxation for region ν

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Applications beyond
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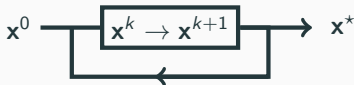
1st-order methods

Proximal gradient

Coordinate descent

...

iteration



Axis 2 – Convex optimization

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Applications beyond
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1st-order methods

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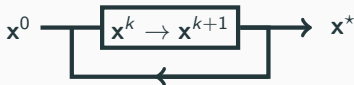
Solving cost

cost per iteration

×

number of iterations

iteration



Axis 2 – Convex optimization

Relaxation for region ν

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Applications beyond
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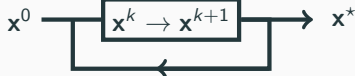
1st-order methods

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Solving cost

cost per iteration

×

number of iterations

dimension of \mathbf{x}

Axis 2 – Convex optimization

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Applications beyond
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1st-order methods

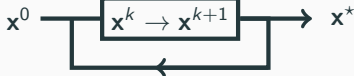
Proximal gradient

Coordinate descent

...

iteration

$$\mathbf{x}^k \rightarrow \mathbf{x}^{k+1}$$



Solving cost

cost per iteration

×

number of iterations

dimension of \mathbf{x}

regularity of f/\tilde{g}

Axis 2 – Sparse structure exploitation

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

Task

Reduce the solving cost

Axis 2 – Sparse structure exploitation

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

Task

Reduce the solving cost



Option 1

Reduce the dimension of \mathbf{x}

Axis 2 – Sparse structure exploitation

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

\tilde{g} non-smooth at $\mathbf{x} = \mathbf{0}$



sparse solution \mathbf{x}^*

Task

Reduce the solving cost



Option 1

Reduce the dimension of \mathbf{x}

Axis 2 – Sparse structure exploitation

Convex problem

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\tilde{g} non-smooth at $\mathbf{x} = \mathbf{0}$



sparse solution \mathbf{x}^*

Task

Reduce the solving cost

Option 1

Reduce the dimension of \mathbf{x}



Screening tests

Identify zeros in \mathbf{x}^*

L. El Ghaoui *et al.* (2011)

E. Ndiaye *et al.* (2020)

Axis 2 – Sparse structure exploitation

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

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Reduce the solving cost

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Option 2

Improve the regularity of f/\tilde{g}

Axis 2 – Sparse structure exploitation

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

\tilde{g} non-smooth at $\mathbf{x} = \mathbf{0}$



sparse solution \mathbf{x}^*

Task

Reduce the solving cost

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Option 2

Improve the regularity of f/\tilde{g}



Smoothing tests

Identify non-zeros in \mathbf{x}^*

Axis 2 – Sparse structure exploitation

Convex problem

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\tilde{g} non-smooth at $\mathbf{x} = \mathbf{0}$



sparse solution \mathbf{x}^*

Task

Reduce the solving cost

Option 1

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Smoothing tests

Identify non-zeros in \mathbf{x}^*



Axis 2 – Screening and smoothing tests

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

Axis 2 – Screening and smoothing tests

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

Dual problem

$$\max_{\mathbf{u} \in \mathbb{R}^m} D(\mathbf{u})$$

Axis 2 – Screening and smoothing tests

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

solution \mathbf{x}^*



if strong duality holds

$$\mathbf{A}^T \mathbf{u}^* \in \partial \tilde{g}(\mathbf{x}^*)$$



solution \mathbf{u}^*

Dual problem

$$\max_{\mathbf{u} \in \mathbb{R}^m} D(\mathbf{u})$$

Axis 2 – Screening and smoothing tests

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

solution \mathbf{x}^*



if strong duality holds

$$\mathbf{A}^T \mathbf{u}^* \in \partial \tilde{g}(\mathbf{x}^*)$$



solution \mathbf{u}^*

Dual problem

$$\max_{\mathbf{u} \in \mathbb{R}^m} D(\mathbf{u})$$

Intermediate result

Some zeros and non-zeros in \mathbf{x}^* can be identified from a dual solution \mathbf{u}^* .

Axis 2 – Screening and smoothing tests

Convex problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

solution \mathbf{x}^*



if strong duality holds

$$\mathbf{A}^T \mathbf{u}^* \in \partial \tilde{g}(\mathbf{x}^*)$$



solution \mathbf{u}^*

Dual problem

$$\max_{\mathbf{u} \in \mathbf{R}^m} D(\mathbf{u})$$

Intermediate result

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Safe region

$$\mathcal{R} \subseteq \mathbf{R}^m \text{ with } \mathbf{u}^* \in \mathcal{R}$$

Axis 2 – Screening and smoothing tests

Convex problem

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if strong duality holds

$$\mathbf{A}^T \mathbf{u}^* \in \partial \tilde{g}(\mathbf{x}^*)$$

solution \mathbf{u}^*

Dual problem

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Intermediate result

Some zeros and non-zeros in \mathbf{x}^* can be identified from a dual solution \mathbf{u}^* .

Safe region

$$\mathcal{R} \subseteq \mathbf{R}^m \text{ with } \mathbf{u}^* \in \mathcal{R}$$

Spotlight result

Some zeros and non-zeros in \mathbf{x}^* can be identified from a safe region \mathcal{R} .

Axis 2 – Screening and smoothing tests

remind $\tilde{g}(\mathbf{x}) = \sum_{i=1}^n \tilde{g}_i(x_i)$

Convex problem

$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

solution \mathbf{x}^*

if strong duality holds

$$\mathbf{A}^T \mathbf{u}^* \in \partial \tilde{g}(\mathbf{x}^*)$$

solution \mathbf{u}^*

Dual problem

$$\max_{\mathbf{u} \in \mathbf{R}^m} D(\mathbf{u})$$

Intermediate result

Some zeros and non-zeros in \mathbf{x}^* can be identified from a dual solution \mathbf{u}^* .

Safe region

$$\mathcal{R} \subseteq \mathbf{R}^m \text{ with } \mathbf{u}^* \in \mathcal{R}$$

Spotlight result

Some zeros and non-zeros in \mathbf{x}^* can be identified from a safe region \mathcal{R} .

Axis 2 – Screening and smoothing tests

remind $\tilde{g}(\mathbf{x}) = \sum_{i=1}^n \tilde{g}_i(x_i)$

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

solution \mathbf{x}^*

if strong duality holds

$$\mathbf{A}^T \mathbf{u}^* \in \partial \tilde{g}(\mathbf{x}^*)$$

solution \mathbf{u}^*

Dual problem

$$\max_{\mathbf{u} \in \mathbb{R}^m} D(\mathbf{u})$$

Intermediate result

Some zeros and non-zeros in \mathbf{x}^* can be identified from a dual solution \mathbf{u}^* .

Safe region

$$\mathcal{R} \subseteq \mathbb{R}^m \text{ with } \mathbf{u}^* \in \mathcal{R}$$

Spotlight result

Some zeros and non-zeros in \mathbf{x}^* can be identified from a safe region \mathcal{R} .

Theorem – Given a safe region \mathcal{R} , note $\mathbf{a}^T \mathcal{R} = \{\mathbf{a}^T \mathbf{u} \mid \mathbf{u} \in \mathcal{R}\}$, one has

$$\text{Screening test: } \mathbf{a}_i^T \mathcal{R} \subseteq \text{int}(\partial \tilde{g}_i(0)) \implies x_i^* = 0$$

$$\text{Smoothing test: } \mathbf{a}_i^T \mathcal{R} \subseteq \text{cpl}(\partial \tilde{g}_i(0)) \implies x_i^* \neq 0$$

Axis 2 – Screening and smoothing tests

remind $\tilde{g}(\mathbf{x}) = \sum_{i=1}^n \tilde{g}_i(x_i)$

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

solution \mathbf{x}^*

if strong duality holds

$$\mathbf{A}^T \mathbf{u}^* \in \partial \tilde{g}(\mathbf{x}^*)$$

solution \mathbf{u}^*

Dual problem

$$\max_{\mathbf{u} \in \mathbb{R}^m} D(\mathbf{u})$$

Intermediate result

Some zeros and non-zeros in \mathbf{x}^* can be identified from a dual solution \mathbf{u}^* .

Safe region

$$\mathcal{R} \subseteq \mathbb{R}^m \text{ with } \mathbf{u}^* \in \mathcal{R}$$

Spotlight result

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Screening test: $\mathbf{a}_i^T \mathcal{R} \subseteq \text{int}(\partial \tilde{g}_i(0)) \implies x_i^* = 0$

Smoothing test: $\mathbf{a}_i^T \mathcal{R} \subseteq \text{cpl}(\partial \tilde{g}_i(0)) \implies x_i^* \neq 0$

easy to evaluate if \mathcal{R} has a simple shape

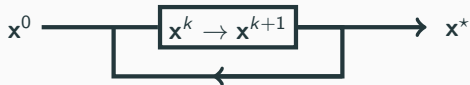
Axis 2 – Dynamic identification

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

1st-order methods

iteration



Axis 2 – Dynamic identification

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

Solving cost

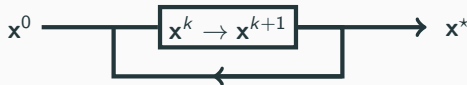
cost per iteration

×

number of iterations

1st-order methods

iteration



Axis 2 – Dynamic identification

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

Solving cost

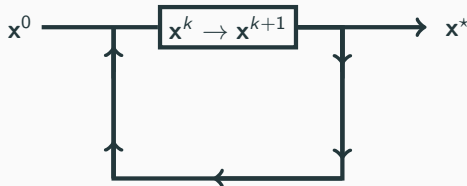
cost per iteration

×

number of iterations

1st-order methods

iteration



Axis 2 – Dynamic identification

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

Solving cost

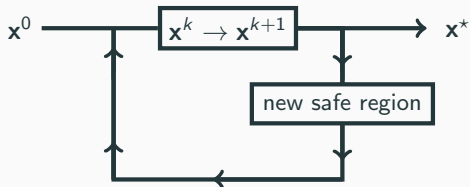
cost per iteration

×

number of iterations

1st-order methods

iteration



Axis 2 – Dynamic identification

Convex problem

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Solving cost

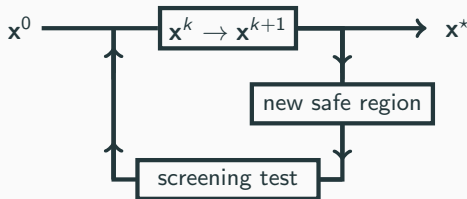
cost per iteration

×

number of iterations

1st-order methods

iteration



Identify some $x_i^* = 0$

Axis 2 – Dynamic identification

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

Solving cost

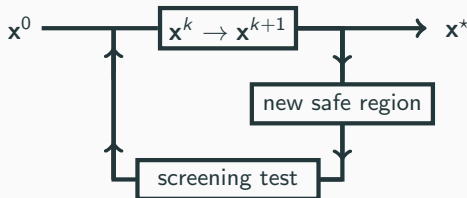
cost per iteration

×

number of iterations

1st-order methods

iteration



Identify some $x_i^* = 0$



Set $x_i = 0$

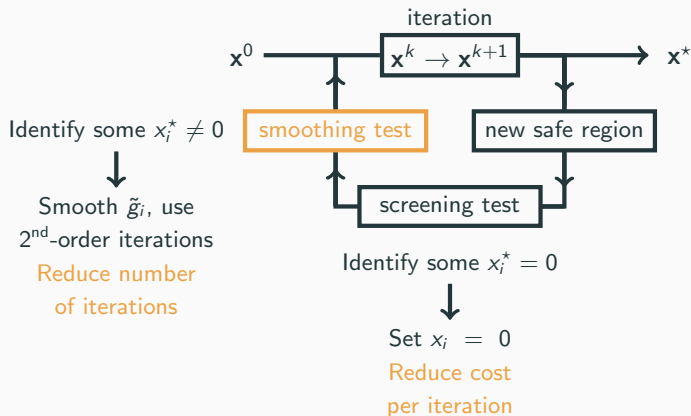
Reduce cost
per iteration

Axis 2 – Dynamic identification

Convex problem
$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

Solving cost
cost per iteration
 \times
number of iterations

1st-order methods

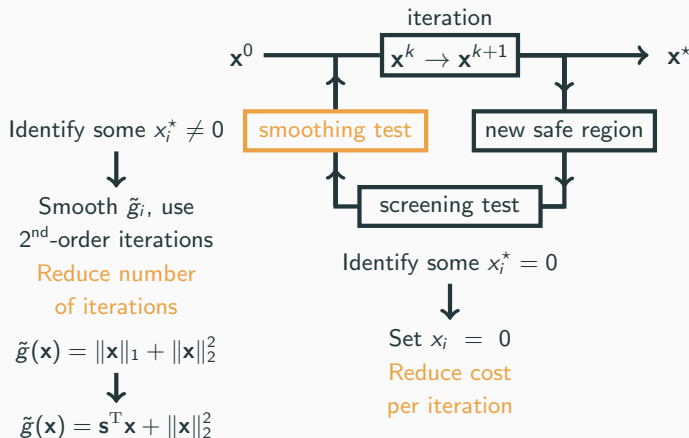


Axis 2 – Dynamic identification

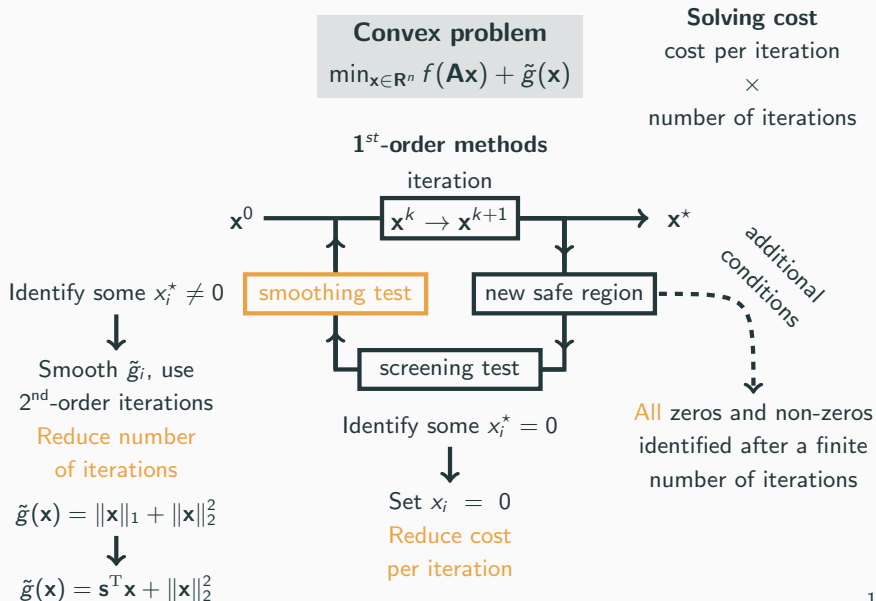
Convex problem
$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

Solving cost
cost per iteration
 \times
number of iterations

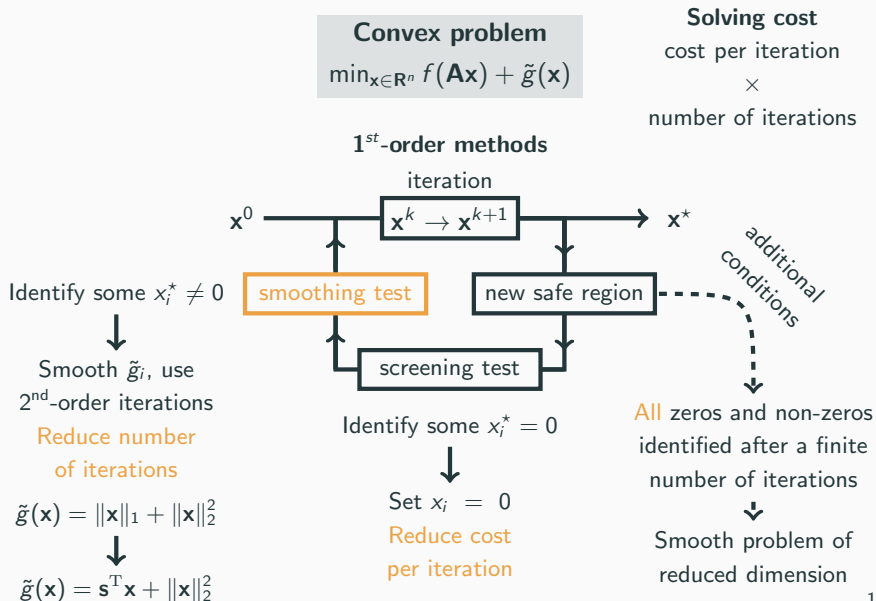
1st-order methods



Axis 2 – Dynamic identification



Axis 2 – Dynamic identification



Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

$$\mathbf{A} \in \mathbb{R}^{100 \times 300} / f : \text{Logistic} / \tilde{g} : \text{Elastic-net}$$

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

$\mathbf{A} \in \mathbb{R}^{100 \times 300}$ / f : Logistic / \tilde{g} : Elastic-net

Accelerated proximal gradient

— Vanilla method

— With screening

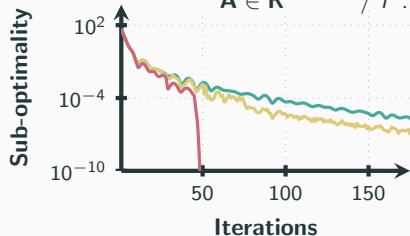
— With screening and smoothing

Axis 2 – Numerics

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

$\mathbf{A} \in \mathbb{R}^{100 \times 300}$ / f : Logistic / \tilde{g} : Elastic-net



Accelerated proximal gradient

— Vanilla method

— With screening

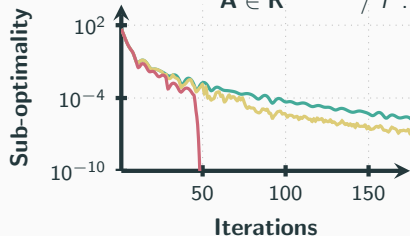
— With screening and smoothing

Axis 2 – Numerics

Convex problem

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Accelerated proximal gradient

— Vanilla method

— With screening

— With screening and smoothing

1st-order \rightarrow 2nd-order

Faster convergence

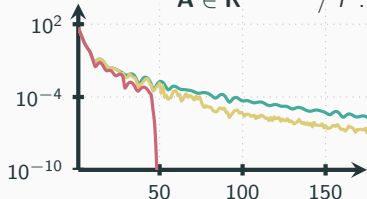
Axis 2 – Numerics

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

$\mathbf{A} \in \mathbb{R}^{100 \times 300}$ / f : Logistic / \tilde{g} : Elastic-net

Sub-optimality



Accelerated proximal gradient

— Vanilla method

— With screening

— With screening and smoothing

Iteration cost



1st-order \rightarrow 2nd-order

Faster convergence

More expensive iterations

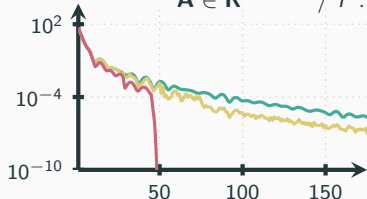
Axis 2 – Numerics

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

$\mathbf{A} \in \mathbb{R}^{100 \times 300}$ / f : Logistic / \tilde{g} : Elastic-net

Sub-optimality



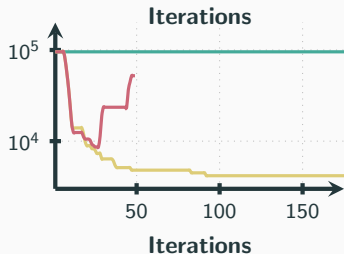
Accelerated proximal gradient

— Vanilla method

— With screening

— With screening and smoothing

Iteration cost



1st-order \rightarrow 2nd-order

Faster convergence

More expensive iterations

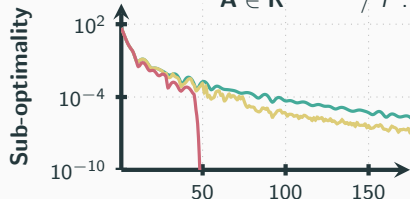
What about the solving time ?

Axis 2 – Numerics

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

$\mathbf{A} \in \mathbb{R}^{100 \times 300}$ / f : Logistic / \tilde{g} : Elastic-net

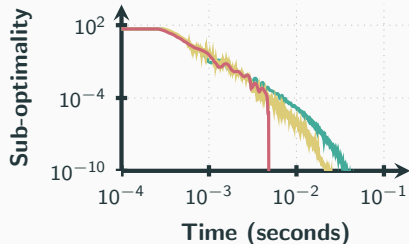


Accelerated proximal gradient

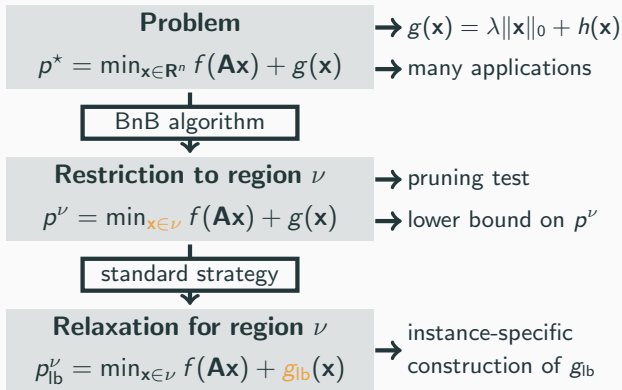
— Vanilla method

— With screening

— With screening and smoothing



Let's recap



Axis 1

How to construct relaxations generically ?

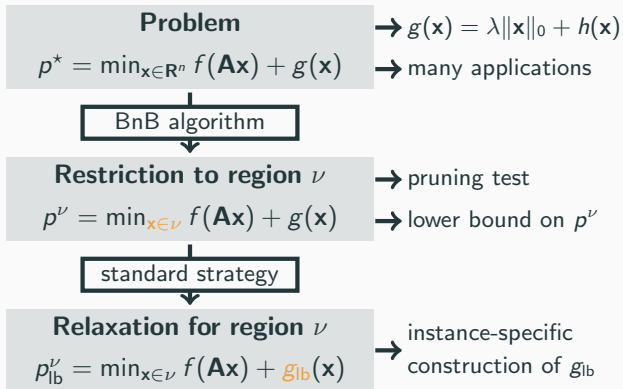
- 1) Set $g_{\text{lb}} = g_{\text{cvx}}$
- 2) Closed-form expression
- 3) Generalize BnB method

Axis 2

How to solve relaxations efficiently ?

- 1) Cast as convex problem
- 2) Screening/smoothing
- 3) Reduce solving cost

Let's recap



Axis 1

How to construct relaxations generically ?

- 1) Set $g_{\text{lb}} = g_{\text{cvx}}$
- 2) Closed-form expression
- 3) Generalize BnB method

Axis 2

How to solve relaxations efficiently ?

- 1) Cast as convex problem
- 2) Screening/smoothing
- 3) Reduce solving cost

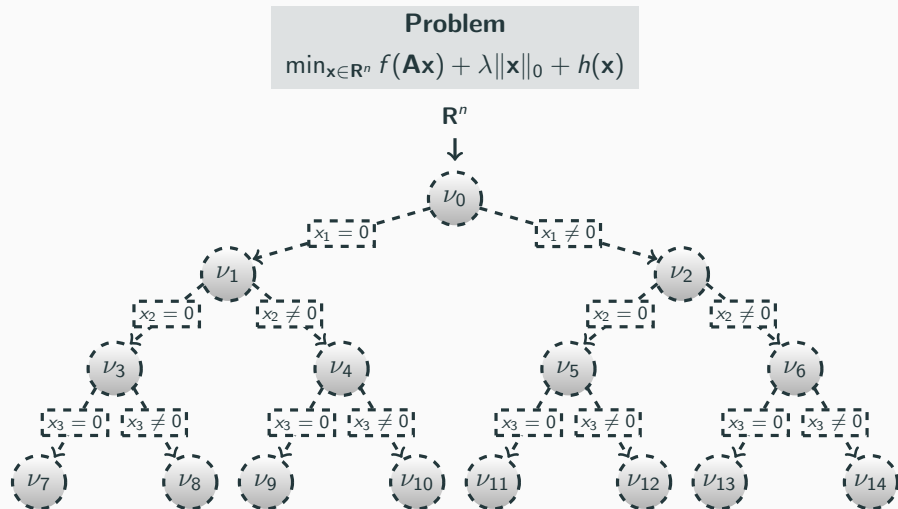
Axis 3

How to improve the standard strategy ?

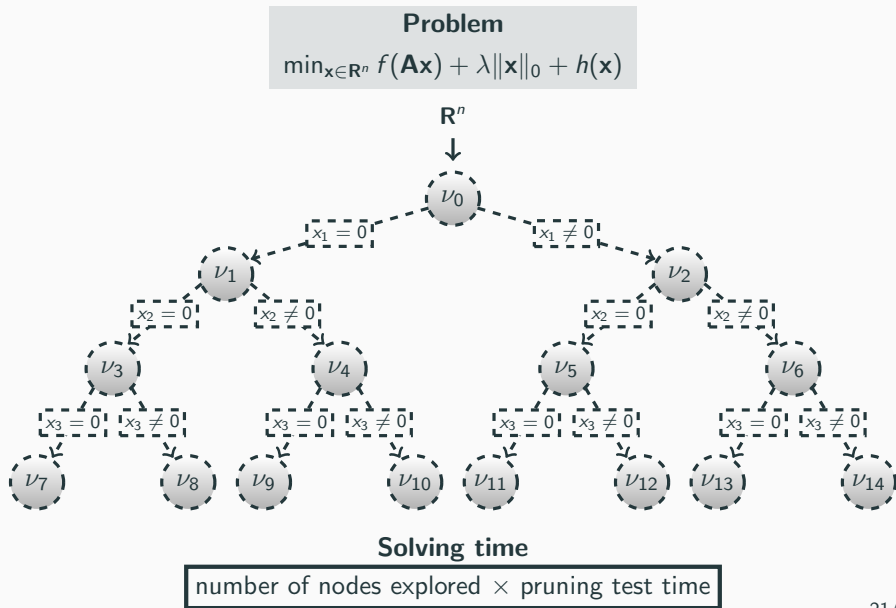
- Manuscript – Chap. 4-5
- ICASSP (2022)
 - EUSIPCO (2023)
 - ICML (2024)

Axis 3 – How to improve the standard strategy ?

Axis 3 – Algorithmic complexity



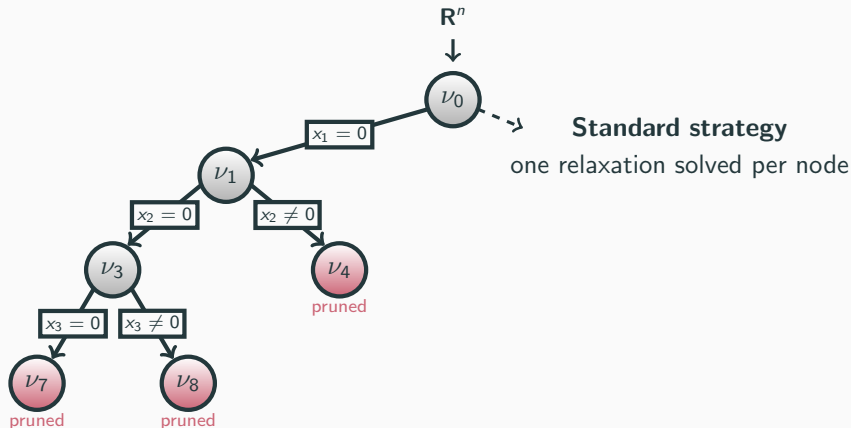
Axis 3 – Algorithmic complexity



Axis 3 – Algorithmic complexity

Problem

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



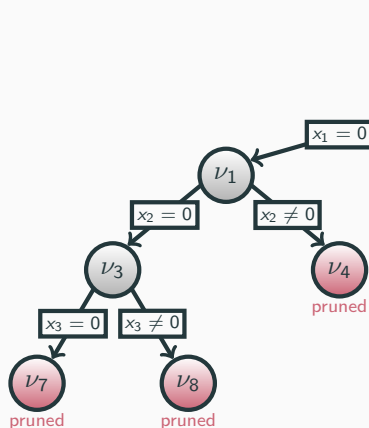
Solving time

number of nodes explored \times pruning test time

Axis 3 – Algorithmic complexity

Problem

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



Standard strategy
one relaxation solved per node

ν_1 and ν_3
processed but
not pruned

↓
useless relaxation
resolution

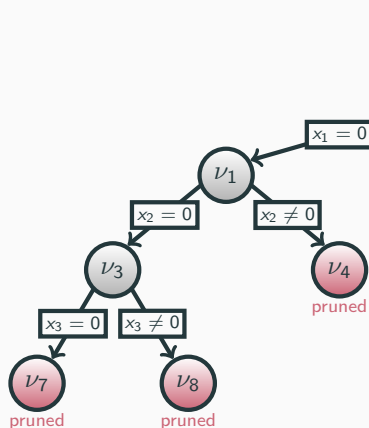
Solving time

number of nodes explored \times pruning test time

Axis 3 – Algorithmic complexity

Problem

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



Standard strategy

one relaxation solved per node

ν_1 and ν_3
processed but
not pruned

↓
useless relaxation
resolution

ν_4 , ν_7 and ν_8
pruned with **rough**
lower bounds

↓
unnecessarily tight
lower bounds

Solving time

number of nodes explored × pruning test time

Axis 3 – Dual bounds

Question

Can we balance the **complexity/tightness** tradeoff when computing the lower bound on p^ν ?

Restriction to region ν

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

$$\rightarrow g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

Axis 3 – Dual bounds

Question

Can we balance the **complexity/tightness** tradeoff when computing the lower bound on p^ν ?

standard strat.

Restriction to region ν

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

$$\rightarrow g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

\vee

Relaxation for region ν

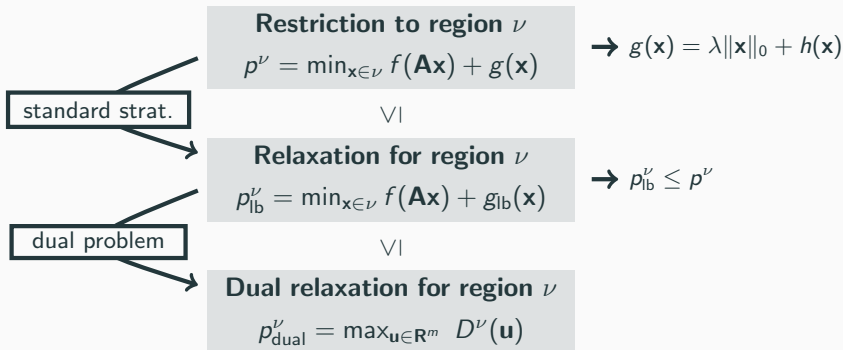
$$p_{\text{lb}}^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{lb}}(\mathbf{x})$$

$$\rightarrow p_{\text{lb}}^\nu \leq p^\nu$$

Axis 3 – Dual bounds

Question

Can we balance the **complexity/tightness** tradeoff when computing the lower bound on p^ν ?



Axis 3 – Dual bounds

Question

Can we balance the **complexity/tightness** tradeoff when computing the lower bound on p^ν ?

standard strat.

Restriction to region ν

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

$$\rightarrow g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

\vee

Relaxation for region ν

$$p_{\text{lb}}^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{lb}}(\mathbf{x})$$

$$\rightarrow p_{\text{lb}}^\nu \leq p^\nu$$

\vee

dual problem

Dual relaxation for region ν

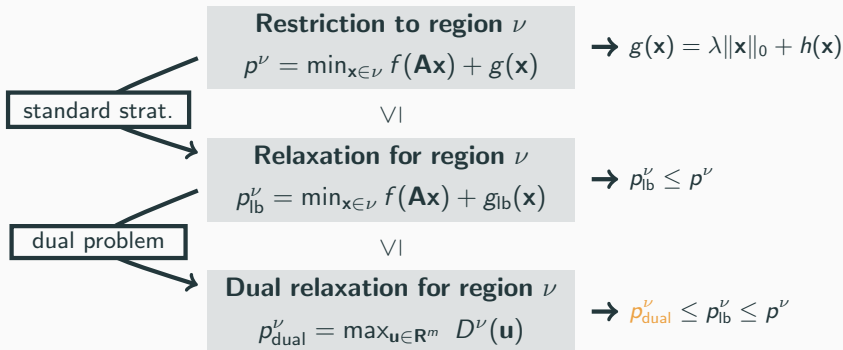
$$p_{\text{dual}}^\nu = \max_{\mathbf{u} \in \mathbf{R}^m} D^\nu(\mathbf{u})$$

$$\rightarrow p_{\text{dual}}^\nu \leq p_{\text{lb}}^\nu \leq p^\nu$$

Axis 3 – Dual bounds

Question

Can we balance the **complexity/tightness** tradeoff when computing the lower bound on p^ν ?



Any evaluation of D^ν gives a lower-bound on p^ν

Axis 3 – Successor link

Standard lower bound

$$p^\nu \geq p_{\text{lb}}^\nu$$

Tight but expensive

Dual lower bound

$$p^\nu \geq D^\nu(\mathbf{u})$$

Rough but economical

Axis 3 – Successor link

Standard lower bound

$$p^\nu \geq p_{\text{lb}}^\nu$$

Tight but expensive

A. Atamtürk *et al.* (2020) / G. Samain *et al.* (2023)

Dual lower bound

$$p^\nu \geq D^\nu(\mathbf{u})$$

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A. Atamtürk *et al.* (2020) / G. Samain *et al.* (2023)

Dual lower bound

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Spotlight result

Successor nodes in the BnB tree share similar dual lower bounds.

Axis 3 – Successor link

Standard lower bound

$$p^\nu \geq p_{\text{lb}}^\nu$$

Tight but expensive

Dual lower bound

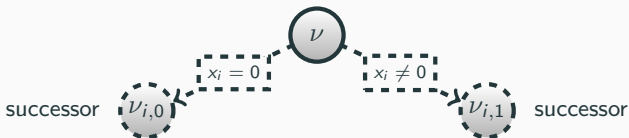
$$p^\nu \geq D^\nu(\mathbf{u})$$

Rough but economical

A. Atamtürk *et al.* (2020) / G. Samain *et al.* (2023)

Spotlight result

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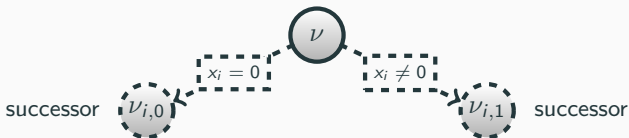
$$p^\nu \geq D^\nu(\mathbf{u})$$

Rough but economical

A. Atamtürk *et al.* (2020) / G. Samain *et al.* (2023)

Spotlight result

Successor nodes in the BnB tree share similar dual lower bounds.



Theorem – Let $\nu_{i,b}$ with $b \in \{0, 1\}$ be a successor of node ν , then

$$D^{\nu_{i,b}}(\mathbf{u}) = D^\nu(\mathbf{u}) + \Delta^{i,b}(\mathbf{u})$$

Axis 3 – Successor link

Standard lower bound

$$p^\nu \geq p_{\text{lb}}^\nu$$

Tight but expensive

Dual lower bound

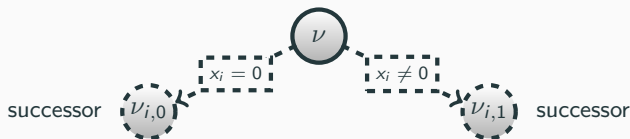
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A. Atamtürk *et al.* (2020) / G. Samain *et al.* (2023)

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Independent of $\nu_{i,b}$

Virtually cost-free

Axis 3 – Successor link

Standard lower bound

$$p^\nu \geq p_{\text{lb}}^\nu$$

Tight but expensive

Dual lower bound

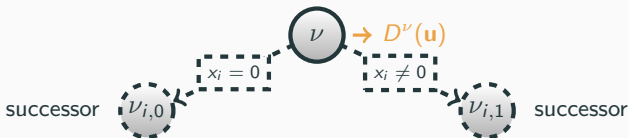
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Independent of $\nu_{i,b}$

Virtually cost-free

Axis 3 – Successor link

Standard lower bound

$$p^\nu \geq p_{\text{lb}}^\nu$$

Tight but expensive

Dual lower bound

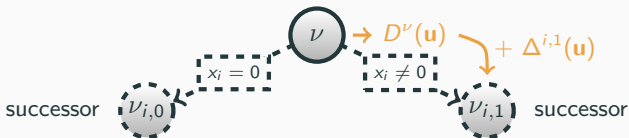
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Independent of $\nu_{i,b}$

Virtually cost-free

Axis 3 – Paradigm shift

Standard pruning

Solve one relaxation per node

Select **two successors** to test next

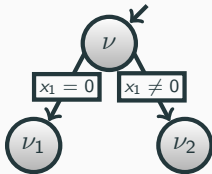


Axis 3 – Paradigm shift

Standard pruning

Solve one relaxation per node

Select **two successors** to test next

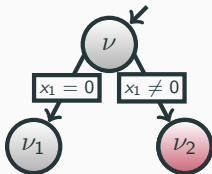


Axis 3 – Paradigm shift

Standard pruning

Solve one relaxation per node

Select **two successors** to test next

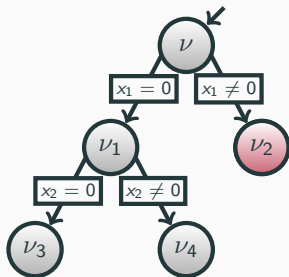


Axis 3 – Paradigm shift

Standard pruning

Solve one relaxation per node

Select **two successors** to test next

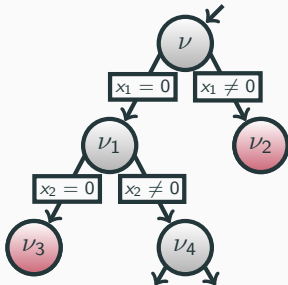


Axis 3 – Paradigm shift

Standard pruning

Solve one relaxation per node

Select **two successors** to test next

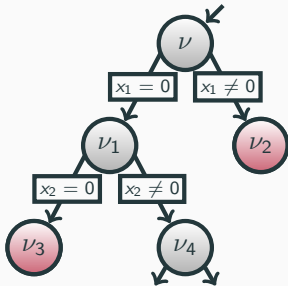


Axis 3 – Paradigm shift

Standard pruning

Solve one relaxation per node

Select **two successors** to test next

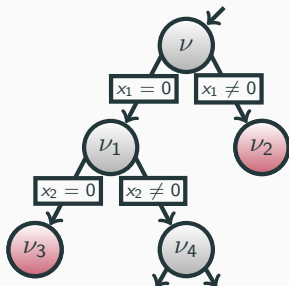


Slow and costly
tree expansion

Axis 3 – Paradigm shift

Standard pruning

Solve one relaxation per node
Select **two successors** to test next



Slow and costly
tree expansion

Simultaneous pruning

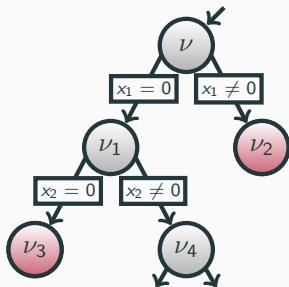
Obtain $D^\nu(\mathbf{u})$ during node processing
Test **all successors** with dual bounds



Axis 3 – Paradigm shift

Standard pruning

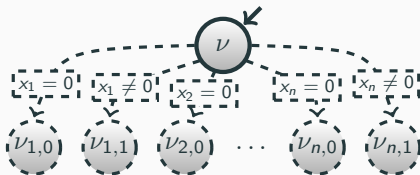
Solve one relaxation per node
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Slow and costly
tree expansion

Simultaneous pruning

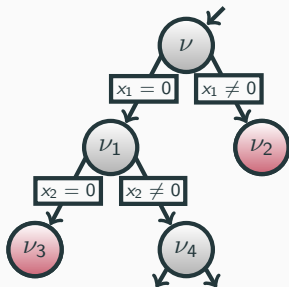
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Standard pruning

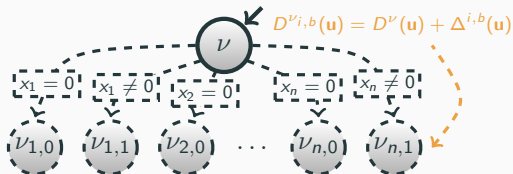
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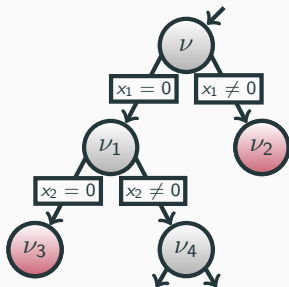
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Standard pruning

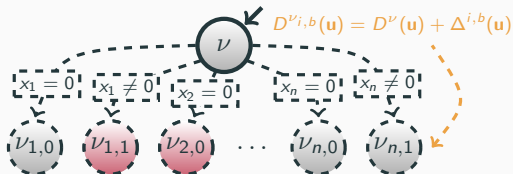
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Simultaneous pruning

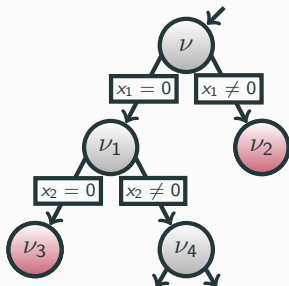
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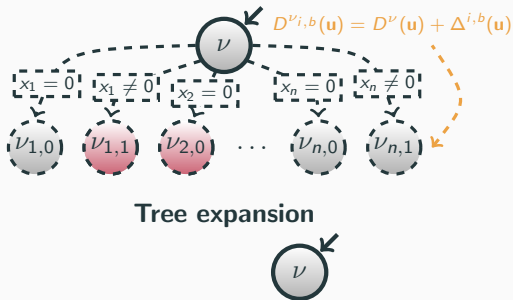
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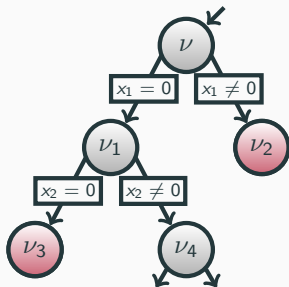
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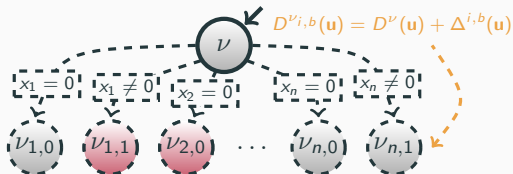
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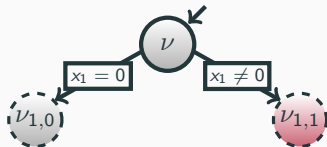
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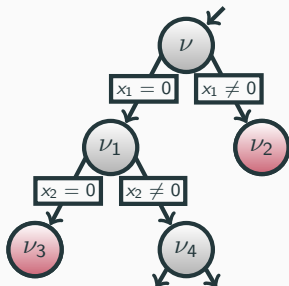
Tree expansion



Axis 3 – Paradigm shift

Standard pruning

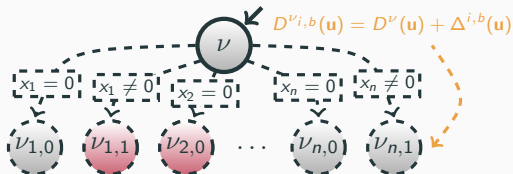
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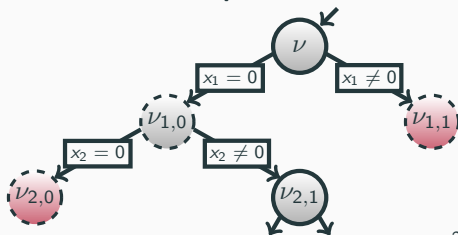
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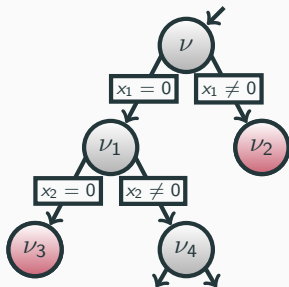
Tree expansion



Axis 3 – Paradigm shift

Standard pruning

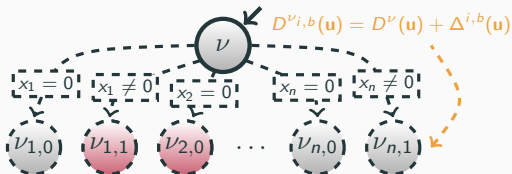
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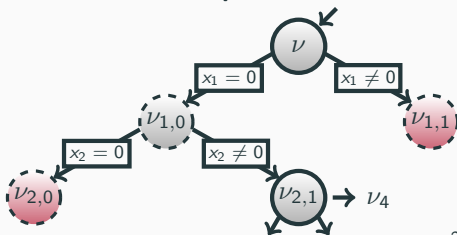
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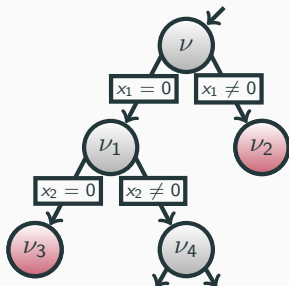
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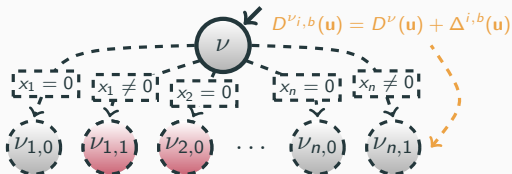
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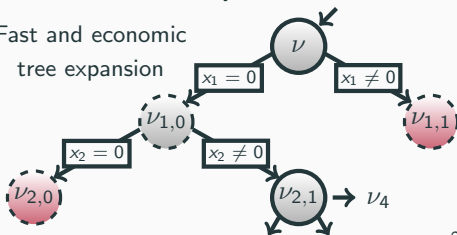
Simultaneous pruning

Obtain $D^\nu(\mathbf{u})$ during node processing
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Tree expansion

Fast and economic
tree expansion



Problem

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

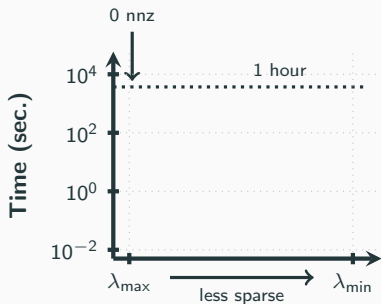
$\mathbf{A} \in \mathbb{R}^{62 \times 2000}$ from ML dataset / f : Logistic / h : ℓ_2 -norm

Axis 3 – Numerics

Problem

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

$\mathbf{A} \in \mathbb{R}^{62 \times 2000}$ from ML dataset / f : Logistic / h : ℓ_2 -norm

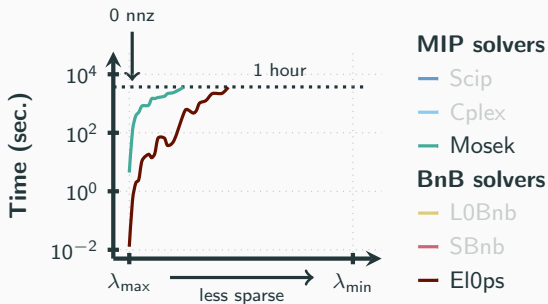


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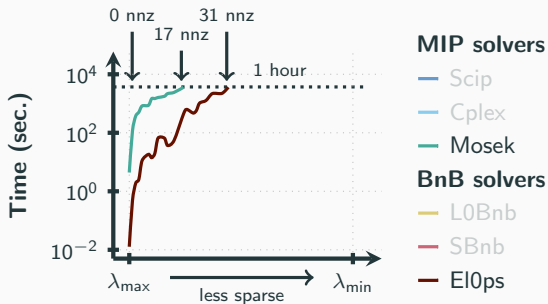


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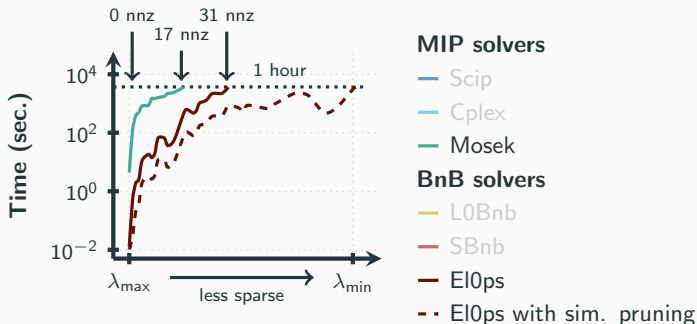


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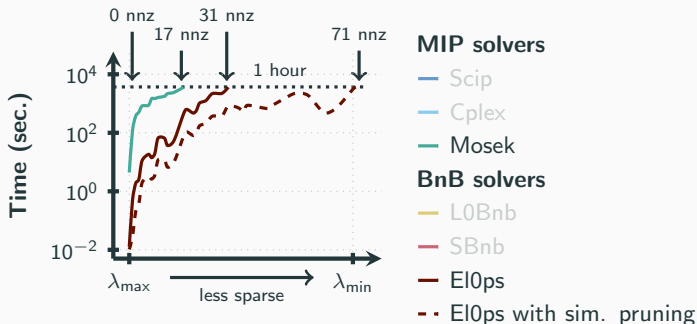


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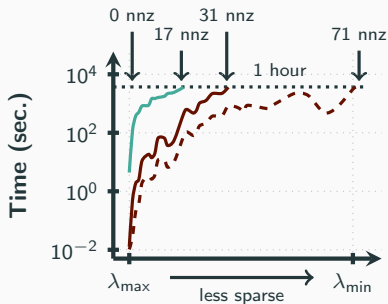


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MIP solvers

— Scip
— Cplex
— Mosek

BnB solvers

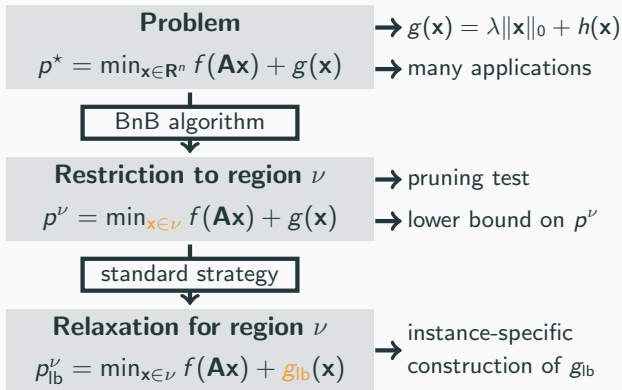
— L0Bnb
— SBnb
— EI0ps
- - EI0ps with sim. pruning

Faster solving time



New sparsity regimes

Let's recap



Axis 1

How to construct relaxations generically ?

- 1) Set $g_{\text{lb}} = g_{\text{cvx}}$
- 2) Closed-form expression
- 3) Generalize BnB method

Axis 2

How to solve relaxations efficiently ?

- 1) Cast as convex problem
- 2) Screening/smoothing
- 3) Accelerate solution

Axis 3

How to improve the standard strategy ?

- 1) Dual bound $D^\nu(\mathbf{u}) \leq p^\nu$
- 2) Link between successors
- 3) Change of paradigm

Conclusion

Problem

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

minimize loss / sparse solutions

Problem

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

minimize loss / sparse solutions

Question

How to design **generic** and **efficient** solution methods ?

Problem

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

minimize loss / sparse solutions

Question

How to design **generic** and **efficient** solution methods ?

1) Generic solver

Axis 1

BnB solver with
generic framework

Problem

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

minimize loss / sparse solutions

Question

How to design **generic** and **efficient** solution methods ?

1) Generic solver

Axis 1

BnB solver with
generic framework

2) Efficient solver

Axis 2 & 3

Efficient relaxation solu-
tion, simultaneous pruning

Problem

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

minimize loss / sparse solutions

Question

How to design **generic** and **efficient** solution methods ?

1) Generic solver

Axis 1

BnB solver with
generic framework

2) Efficient solver

Axis 2 & 3

Efficient relaxation solu-
tion, simultaneous pruning

3) Practical solver

El0ps

Flexible with state-of-
the-art performance

Extension to other formulations

Minimize loss $f(\mathbf{Ax})$

Force sparsity with $\|\mathbf{x}\|_0$



contributions

Regularized version

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

Perspectives

Extension to other formulations

Minimize loss $f(\mathbf{Ax})$

Force sparsity with $\|\mathbf{x}\|_0$

contributions

```
graph TD; A[contributions] --> B[Regularized version]; C[connections] --> B; B --> D[Constrained version];
```

Regularized version

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

connections

Constrained version

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) \text{ s.t. } \|\mathbf{x}\|_0 \leq k$$

Perspectives

Extension to other formulations

Minimize loss $f(\mathbf{Ax})$

Force sparsity with $\|\mathbf{x}\|_0$

contributions

```
graph TD; A["Minimize loss f(Ax)  
Force sparsity with ||x||_0"] --> B[contributions]; B --> C["Regularized version  
min_{x in R^n} f(Ax) + lambda ||x||_0"]; C --> D[connections]; D --> E["Constrained version  
min_{x in R^n} f(Ax) s.t. ||x||_0 <= k"]; E --> F["→ non-separability of  
the l_0-norm constraint"];
```

Regularized version

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connections

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→ non-separability of
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Towards stronger relaxations

Restriction to region ν

$$\min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g(\mathbf{x})$$

lower bound

Convex relaxation

$$\min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{cvx}}(\mathbf{x})$$

Perspectives

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improve

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→ tune $g_{\text{non-cvx}}$ to preserve
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Broader exploitation of smoothing tests

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \tilde{g}(\mathbf{x})$$

accelerate

Screen/smooth tests

$$x_i^* = 0 \text{ or } x_i^* \neq 0$$

Perspectives

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$$x_i^* = 0 \text{ or } x_i^* \neq 0$$

Set $x_i = 0$
Tailored to any instance

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↓
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Tailored to any instance

↓
Smooth \tilde{g}_i
Depends on the instance

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↓ ↓
Set $x_i = 0$ Smooth \tilde{g}_i
Tailored to Depends on
any instance the instance

→ Newton accel. for proximal identification
G. Bareilles *et al.* (2022)

Question time !



Context – Machine learning application

Tabular ML dataset

	Feature 1	Feature 2	...	Feature n	Target
Sample 1	$a_{1,1}$	$a_{1,2}$...	$a_{1,n}$	y_1
Sample 2	$a_{2,1}$	$a_{2,2}$...	$a_{2,n}$	y_2
Sample 3	$a_{3,1}$	$\mathbf{A} \in \mathbb{R}^{m \times n}$...	$a_{3,n}$	$\mathbf{y} \in \mathbb{R}^m$
...
Sample m	$a_{m,1}$	$a_{m,2}$...	$a_{m,n}$	y_m

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

Model accuracy

Loss $\mathcal{L}_\phi(\mathbf{Ax}, \mathbf{y})$



Model explicability

Sparsity-inducing $\mathcal{R}(\mathbf{x})$



Optimization problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} \mathcal{L}_\phi(\mathbf{Ax}, \mathbf{y}) + \lambda \mathcal{R}(\mathbf{x})$$

Context – Algebra application

Sparse Component Analysis

Goal

Given $\mathbf{M} \in \mathbf{R}^{m \times n}$, find $\mathbf{D} \in \mathbf{R}^{m \times r}$ and $\mathbf{B} \in \mathbf{R}^{r \times n}$ such that $\mathbf{M} \simeq \mathbf{DB}$ with **sparse** columns in \mathbf{B} .



Optimization problem

$$\min_{\mathbf{D} \in \mathbf{R}^{m \times r}, \mathbf{B} \in \mathbf{R}^{r \times n}} \frac{1}{2} \|\mathbf{M} - \mathbf{DB}\|_F^2 + \lambda \sum_{i=1}^n \|\mathbf{b}_i\|_0$$

J. Cohen, N. Gillis (2019)

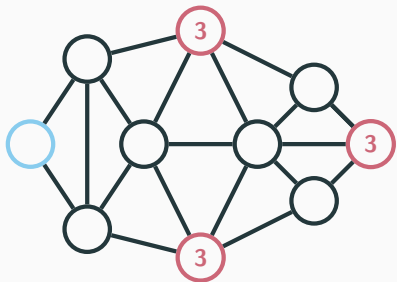


Extract material
abundance map from
hyperspectral image

Context – Operation research application

Max. capacity per edge: 10

Edge construction cost: 5



Which edges to build to transport flows from **source** to **sink** nodes ?

Network design

$$\begin{cases} \min Q(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 \\ \text{s.t. } \mathbf{D}\mathbf{x} \leq \mathbf{d}, \mathbf{x} \leq \mathbf{c} \\ \mathbf{x} \in \mathbf{R}_+^{\text{card}(E)} \end{cases}$$

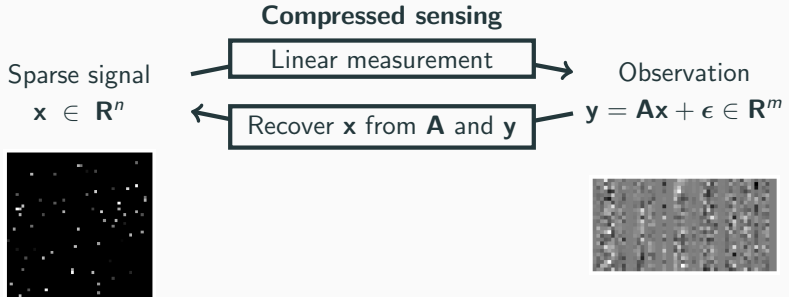
Q : transportation cost

λ : unit construction cost

$\mathbf{D}\mathbf{x} \leq \mathbf{d}$: flow conservation

$\mathbf{x} \leq \mathbf{c}$: capacity constraint

Context – Signal processing application



Goal

Find \mathbf{x} such that $\mathbf{y} \simeq \mathbf{Ax}$

$m \ll n$: no unique solution

Goal (with sparse prior)

Find \mathbf{x} **sparse** such that $\mathbf{y} \simeq \mathbf{Ax}$

Optimization problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} \frac{1}{2} \|\mathbf{y} - \mathbf{Ax}\|_2^2$$

sparsity-inducing function

Sparse optimization problem

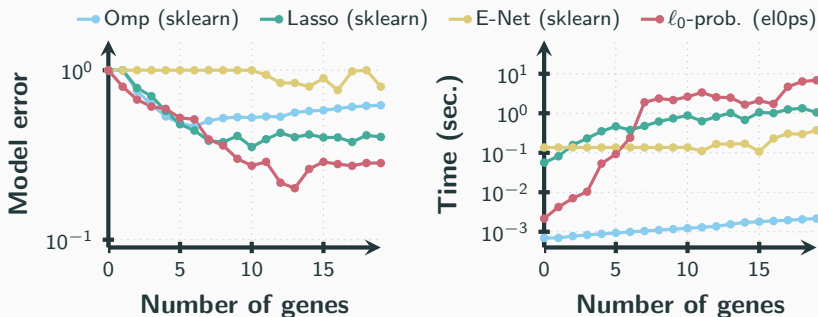
$$\min_{\mathbf{x} \in \mathbb{R}^n} \frac{1}{2} \|\mathbf{y} - \mathbf{Ax}\|_2^2 + \lambda \|\mathbf{x}\|_0$$

Context – 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
#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

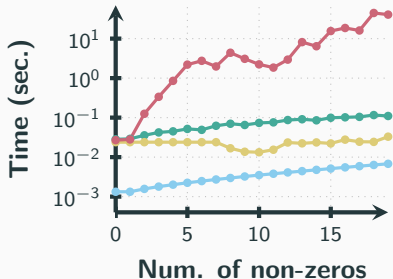
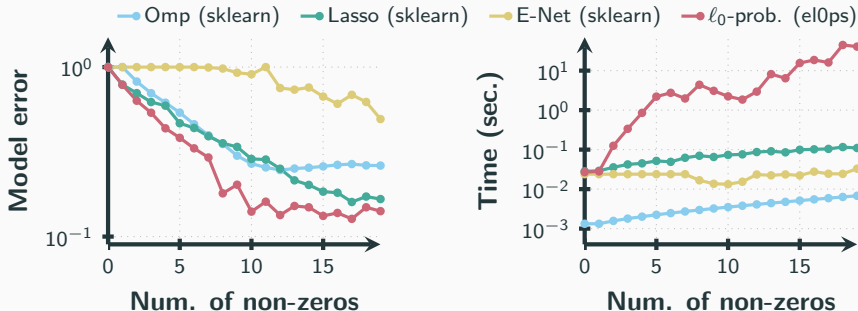
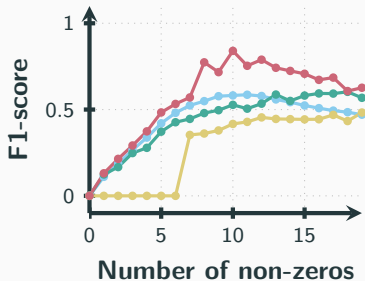


Context – Balancing solution quality and problem hardness



Setup

$\mathbf{A} \in \mathbb{R}^{100 \times 200}$ highly correlated, $\epsilon \sim \mathcal{N}(0, \sigma \mathbf{I})$,
 \mathbf{x} with 10 unit spikes of random location

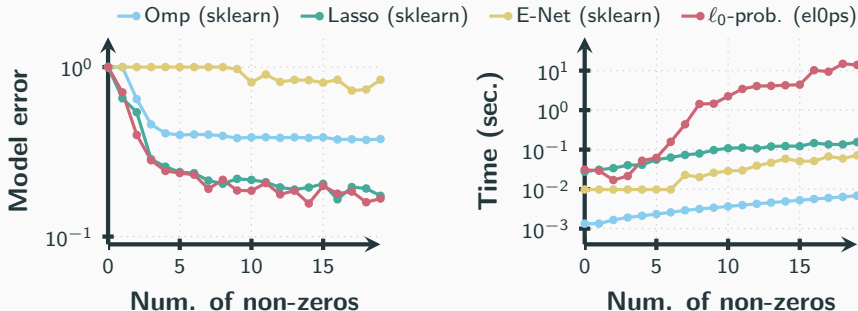
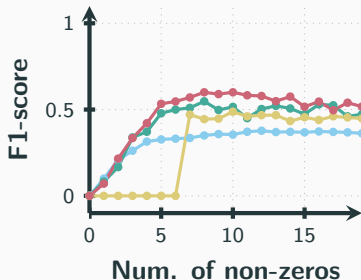


Context – Balancing solution quality and problem hardness



Setup

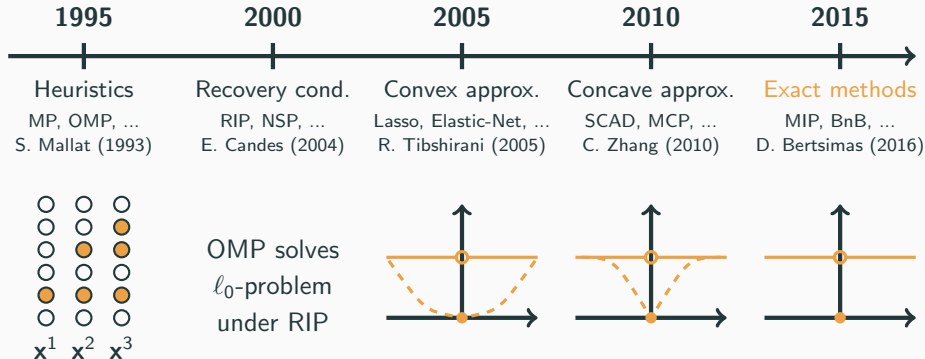
$\mathbf{A} \in \mathbb{R}^{100 \times 200}$ highly correlated, $\epsilon \sim \mathcal{N}(0, \sigma \mathbf{I})$,
 \mathbf{x} with 10 unit and evenly-spaced spikes



Context – A bit of history

Problem

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



Context – MIP formulation

Problem

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

linearize ℓ_0 -norm

MIP formulation

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

avoid logical cstr.

Practical MIP formulation

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

Use generic MIP solvers

Need standardized expressions
linear/quadratic/conic/...

Lifted formulation

$$\|\mathbf{x}\|_0 = \mathbf{1}^T \mathbf{z}$$

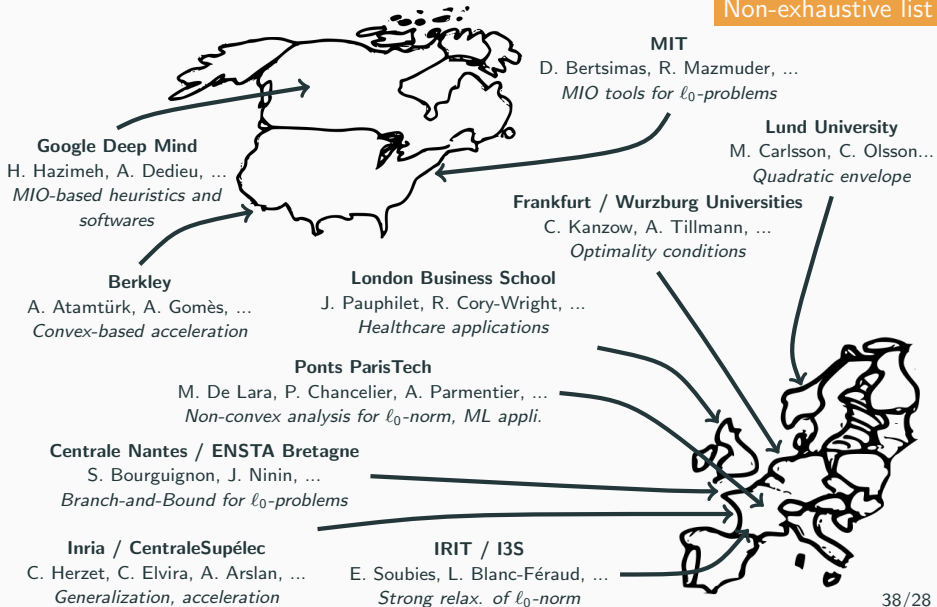
for all $\mathbf{x} \in \mathbf{R}^n$ and $\mathbf{z} \in \{0, 1\}^n$
if $x_i = 0 \implies z_i = 0, \forall i$

Construct h_{mip} depending on h

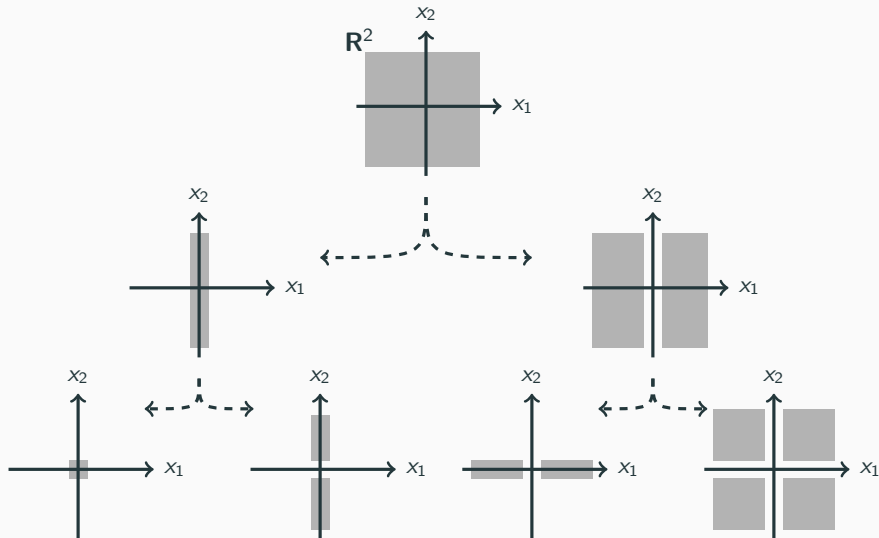
$h(\mathbf{x})$	$h_{\text{mip}}(\mathbf{x}, \mathbf{z})$
$\eta(\ \mathbf{x}\ _\infty \leq M)$	$\eta(-M\mathbf{z} \leq \mathbf{x} \leq M\mathbf{z})$
$\alpha \ \mathbf{x}\ _2^2$	$\sum_{i=1}^n \alpha \frac{x_i^2}{z_i}$

Context – Research community

Non-exhaustive list



BnB – Region separation



Axis 1 – Relaxation construction



$$\text{Region } \nu \equiv (\mathcal{S}_0, \mathcal{S}_1, \mathcal{S}_\bullet) \text{ with } \begin{cases} x_i = 0 & \text{if } i \in \mathcal{S}_0 \\ x_i \neq 0 & \text{if } i \in \mathcal{S}_1 \\ x_i \in \mathbf{R} & \text{if } i \in \mathcal{S}_\bullet \end{cases}$$

Restriction to region ν

$$p^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g(\mathbf{x}) \quad \text{with} \quad g_i(x_i) = \lambda \|x_i\|_0 + h_i(x_i)$$

reformulation

Restriction to region ν

$$p^\nu = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{Ax}) + g^\nu(\mathbf{x}) \quad \text{with} \quad g_i^\nu(x_i) = \begin{cases} g_i(x_i) + \eta(x_i = 0) & \text{if } i \in \mathcal{S}_0 \\ g_i(x_i) + \eta(x_i \neq 0) & \text{if } i \in \mathcal{S}_1 \\ g_i(x_i) & \text{if } i \in \mathcal{S}_\bullet \end{cases}$$

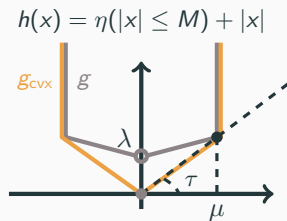
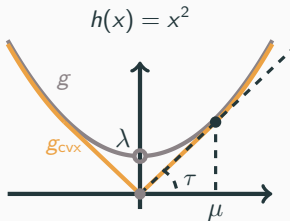
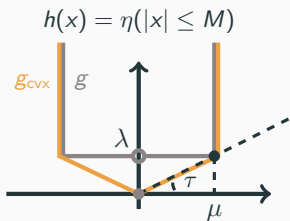
$g_{\text{lb}}^\nu \leq g$, g_{lb}^ν convex

Relaxation for region ν

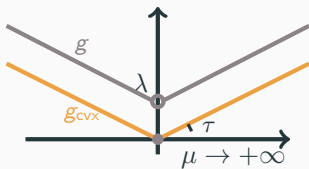
$$p_{\text{lb}}^\nu = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{Ax}) + g_{\text{lb}}^\nu(\mathbf{x}) \quad \text{with} \quad g_{i,\text{lb}}^\nu(x_i) = \begin{cases} \eta(x_i = 0) & \text{if } i \in \mathcal{S}_0 \\ h_i(x_i) + \lambda & \text{if } i \in \mathcal{S}_1 \\ g_{i,\text{cvx}}(x_i) & \text{if } i \in \mathcal{S}_\bullet \end{cases}$$

Axis 1 – Graphical interpretation

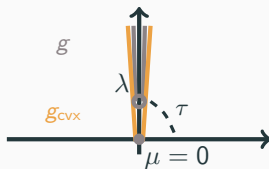
$$g(x) = \lambda \|x\|_0 + h(x) \xrightarrow{\text{convexify}} g_{\text{cvx}}(x) = \begin{cases} \tau |x| & \text{if } |x| \leq \mu \\ \lambda + h(x) & \text{otherwise} \end{cases}$$



$h(x) = |x|$



$h(x) = \eta(x = 0)$



Axis 2 – Reduced and smoothed formulation

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \lambda \|\mathbf{x}\|_1 + h(\mathbf{x})$$

Knowledge of
zeros/positive/negative
entries in the solutions

Reduced/smoothed formulation

$$\min_{\tilde{\mathbf{x}} \in \mathbb{R}^{\tilde{n}}} f(\tilde{\mathbf{A}}\tilde{\mathbf{x}}) + \lambda \boldsymbol{\theta}^T \tilde{\mathbf{x}} + h(\tilde{\mathbf{x}})$$

Reduced dimension $\tilde{n} \ll n$

Smooth objective if f/h smooth

1st-order methods

Proximal gradient

Coordinate descent



Sub-linear/linear convergence rate

Cost $\mathcal{O}(nm)$ per iteration

2nd-order methods

Newton's method

LBFGS



Super-linear convergence rate

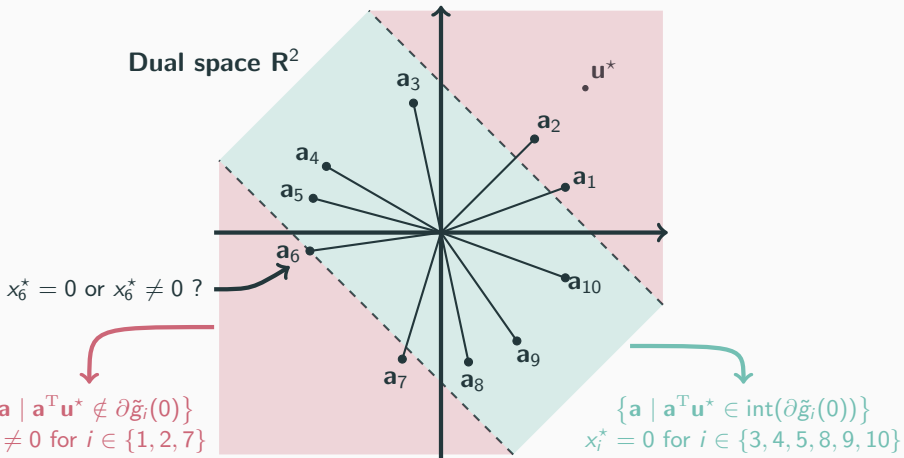
Cost $\mathcal{O}(\tilde{n}m)$ per iteration

Axis 2 – Graphical interpretation (dual)

Screening: $\mathbf{a}_i^T \mathbf{u}^* \in \text{int}(\partial \tilde{g}_i(0)) \implies x_i^* = 0$

Smoothing: $\mathbf{a}_i^T \mathbf{u}^* \in \text{cpl}(\partial \tilde{g}_i(0)) \implies x_i^* \neq 0$

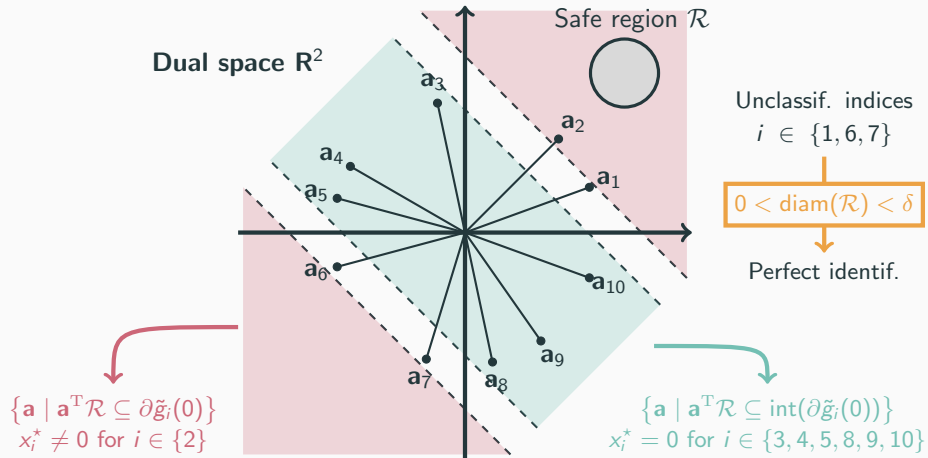
Dual space \mathbb{R}^2



Axis 2 – Graphical interpretation (safe)

Safe screening: $\mathbf{a}_i^T \mathcal{R} \subseteq \text{int}(\partial \tilde{g}_i(0)) \implies x_i^* = 0$

Safe smoothing: $\mathbf{a}_i^T \mathcal{R} \subseteq \text{cpl}(\partial \tilde{g}_i(0)) \implies x_i^* \neq 0$

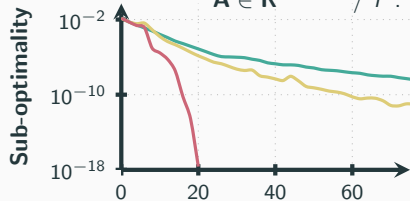


Axis 2 – Numerics

Convex problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

$\mathbf{A} \in \mathbb{R}^{100 \times 300}$ / f : Quadratic / \tilde{g} : $\ell_1 \ell_2$ -norm

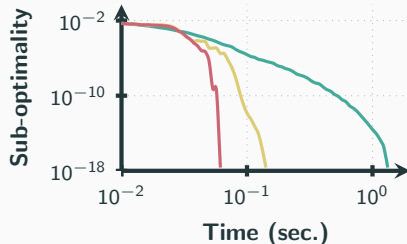
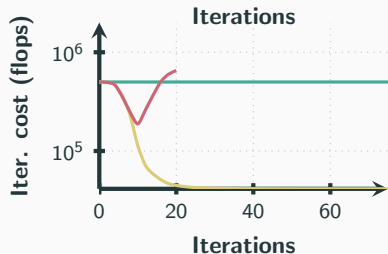


Accelerated proximal gradient

— Vanilla method

— With screening

— With screening and smoothing



Axis 3 – Dual relaxation



$$\text{Region } \nu \equiv (\mathcal{S}_0, \mathcal{S}_1, \mathcal{S}_\bullet) \text{ with } \begin{cases} x_i = 0 & \text{if } i \in \mathcal{S}_0 \\ x_i \neq 0 & \text{if } i \in \mathcal{S}_1 \\ x_i \in \mathbf{R} & \text{if } i \in \mathcal{S}_\bullet \end{cases}$$

Restriction to region ν

$$p^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g(\mathbf{x}) \quad \text{with } g_i(x_i) = \lambda \|x_i\|_0 + h_i(x_i)$$

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

Relaxation for region ν

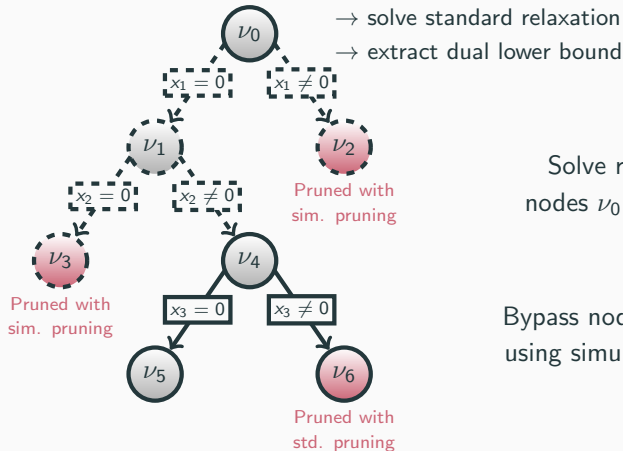
$$p_{\text{lb}}^\nu = \min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{Ax}) + g_{\text{lb}}^\nu(\mathbf{x}) \quad \text{with } g_{i,\text{lb}}^\nu(x_i) = \begin{cases} \eta(x_i = 0) & \text{if } i \in \mathcal{S}_0 \\ h_i(x_i) + \lambda & \text{if } i \in \mathcal{S}_1 \\ g_{i,\text{cvx}}(x_i) & \text{if } i \in \mathcal{S}_\bullet \end{cases}$$

dualize

Dual relaxation for region ν

$$p_{\text{dual}}^\nu = \max_{\mathbf{u} \in \mathbf{R}^m} -f^*(-\mathbf{u}) - (g_{\text{lb}}^\nu)^*(\mathbf{A}^T \mathbf{u}) \quad \text{with } (g_{i,\text{lb}}^\nu)^*(\mathbf{a}_i^T \mathbf{u}) = \begin{cases} 0 & \text{if } i \in \mathcal{S}_0 \\ h_i^*(\mathbf{a}_i^T \mathbf{u}) - \lambda & \text{if } i \in \mathcal{S}_1 \\ [h_i^*(\mathbf{a}_i^T \mathbf{u}) - \lambda]_+ & \text{if } i \in \mathcal{S}_\bullet \end{cases}$$

Axis 3 – Combining both paradigms



Solve relaxations in
nodes ν_0 , ν_4 , ν_5 and ν_6

Bypass nodes ν_1 , ν_2 and ν_3
using simultaneous pruning

Axis 4 – Relaxation strength

Problem

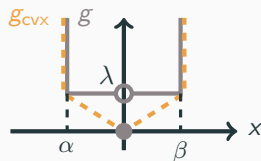
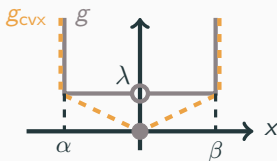
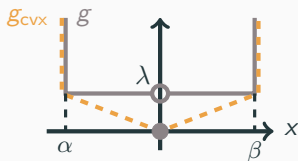
$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{Ax}) + \lambda \|\mathbf{x}\|_0 + \eta(\alpha \leq \mathbf{x} \leq \beta)$$



Pruning test

Construct and solve a relaxation

$$g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + \eta(\alpha \leq \mathbf{x} \leq \beta) \rightarrow g_{\text{cvx}}$$

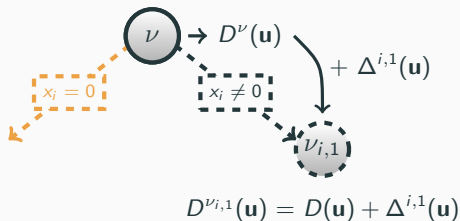


Practical side – Large interval $[\alpha, \beta]$ to obtain relevant solutions.

Numerical side – Small interval $[\alpha, \beta]$ to obtain strong relaxations.

Axis 4 – Peeling tests

Simultaneous pruning test

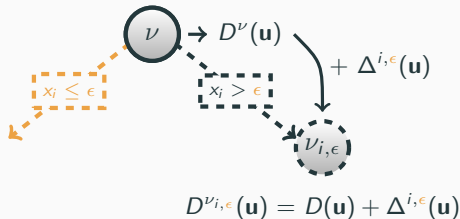


Result 1

→ peeling test gives weaker conclusions but is easier to pass

$$D^{\nu_{i,\epsilon}}(\mathbf{u}) \geq D^{\nu_{i,1}}(\mathbf{u})$$

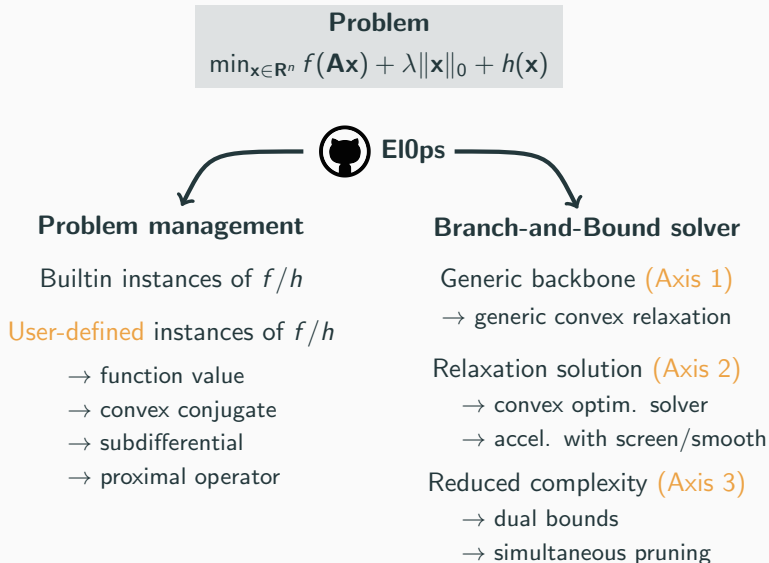
Peeling test



Result 2

→ we can find the smallest $\epsilon > 0$ such that the peeling test is passed

$$\rho_{\text{ub}}^* < D^{\nu_{i,\epsilon}}(\mathbf{u})$$



Perspectives – Stronger relaxations

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

VI

$$p_{\text{non-cvx}}^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{non-cvx}}(\mathbf{x})$$

VI

$$p_{\text{cvx}}^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{Ax}) + g_{\text{cvx}}(\mathbf{x})$$

→ Need valid and tractable relaxation

$$g(\mathbf{x}) = \lambda \|\mathbf{x}\|_0 + \frac{\gamma}{2} \|\mathbf{x}\|_2^2$$

VI

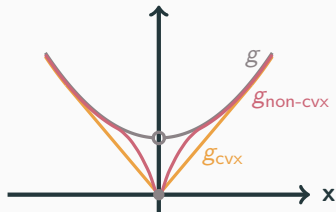
$$g_{\text{non-cvx}}(\mathbf{x}) = \text{Mcp}_{\alpha, \beta}(\mathbf{x}) + \frac{\gamma}{2} \|\mathbf{x}\|_2^2$$

VI

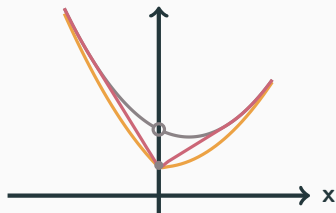
$$g_{\text{cvx}}(\mathbf{x}) = \text{Berhu}_{\lambda, \gamma}(\mathbf{x})$$

→ Tune (α, β) depending on f and \mathbf{A}
to ensure the overall objective convexity

Regularization functions



Objective functions



Perspectives – Proximal identification

Convex problem

$$\mathbf{x}^* \in \operatorname{argmin}_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{A}\mathbf{x}) + \tilde{g}(\mathbf{x})$$

Screening/smoothing

Optimality conditions

$$\mathbf{A}^T \mathbf{u}^* \in \partial \tilde{g}(\mathbf{x}^*)$$

$$\tilde{g}(\mathbf{x}^*) = \sum_{i=1}^n \tilde{g}_i(x_i^*)$$

Identif. from dual solution

$$\mathbf{a}_i^T \mathbf{u}^* \rightarrow x_i^* = 0 \text{ or } x_i^* \neq 0$$

$$\mathcal{R} \subseteq \mathbb{R}^m \text{ with } \mathbf{u}^* \in \mathcal{R}$$

Identif. from safe region

$$\mathbf{a}_i^T \mathcal{R} \rightarrow x_i^* = 0 \text{ or } x_i^* \neq 0$$

Safe but can miss indices

Proximal identification

Optimality conditions

$$\mathbf{x}^* = \operatorname{prox}_{\tilde{g}}(\mathbf{x}^*)$$

$$\tilde{g}(\mathbf{x}^*) = \sum_{i=1}^n \tilde{g}_i(x_i^*)$$

Identif. from prox. operator

$$\operatorname{prox}_{\tilde{g}_i}(x_i^*) \rightarrow x_i^* = 0 \text{ or } x_i^* \neq 0$$

$$\mathbf{x} \in \mathbb{R}^n \text{ near } \mathbf{x}^*$$

Identif. from arbitrary point

$$\operatorname{prox}_{\tilde{g}_i}(x_i) \rightarrow x_i^* = 0 \text{ or } x_i^* \neq 0$$

Unsafe but classify all indices

$$\begin{array}{c} \mathbf{w} = \operatorname{prox}_{\tilde{g}}(\mathbf{x}) \\ \leftarrow \text{dashed arrow} \rightarrow \\ \mathbf{x} - \mathbf{w} \in \partial \tilde{g}(\mathbf{w}) \end{array}$$

unsafe exploit.



Perspectives – Newton acceleration

Algorithm 1: Our approach

Input: $\mathbf{x}^0 \in \mathbb{R}^n$

Initialize $(\mathcal{S}_0, \mathcal{S}_1, \mathcal{S}_\bullet) = (\emptyset, \emptyset, [1, n])$

for $k = 1, 2, \dots, k_{\max}$ do

 // Update iterate

$\mathbf{x}_{\mathcal{S}_0}^k \leftarrow \mathbf{0}$

$\mathbf{x}_{\mathcal{S}_1}^k \leftarrow 2^{\text{nd}}\text{OrderIteration}(\mathbf{x}_{\mathcal{S}_1}^{k-1})$

$\mathbf{x}_{\mathcal{S}_\bullet}^k \leftarrow 1^{\text{st}}\text{OrderIteration}(\mathbf{x}_{\mathcal{S}_\bullet}^{k-1})$

 // Update structure knowledge

$\mathcal{R} \leftarrow \text{SafeRegion}(\mathbf{x}^k)$

$\mathcal{S}_0 \leftarrow \mathcal{S}_0 \cup \text{ScreeningTest}(\mathcal{R})$

$\mathcal{S}_1 \leftarrow \mathcal{S}_1 \cup \text{SmoothingTest}(\mathcal{R})$

$\mathcal{S}_\bullet \leftarrow [1, n] \setminus (\mathcal{S}_0 \cup \mathcal{S}_1)$

end

- $\mathcal{S}_0 \subseteq \mathcal{S}_0^*$ and $\mathcal{S}_1 \subseteq \mathcal{S}_1^*$ at any iter.
- $\mathcal{S}_\bullet \neq \emptyset$ until $k \geq k_0$

→ Safe but **uncomplete** identification

$$\mathcal{S}_0^* = \{i \mid \mathbf{x}_i^* = 0\}$$

$$\mathcal{S}_1^* = \{i \mid \mathbf{x}_i^* \neq 0\}$$

Algorithm 2: G. Bareilles *et al.*

Input: $\mathbf{x}^0 \in \mathbb{R}^n$

for $k = 1, 2, \dots, k_{\max}$ do

 // Update iterate

$\tilde{\mathbf{x}}^k \leftarrow \text{ProxIteration}(\mathbf{x}^{k-1})$

 // Get local structure

$(\mathcal{S}_0, \mathcal{S}_1) \leftarrow \text{ProxIdentification}(\tilde{\mathbf{x}}^k)$

 // Follow local structure

$\mathbf{x}^k \leftarrow \text{StructureUpdate}_{(\mathcal{S}_0, \mathcal{S}_1)}(\tilde{\mathbf{x}}^k)$

end

- $\mathcal{S}_\bullet = \emptyset$ at any iter.
- $\mathcal{S}_0 \neq \mathcal{S}_0^*$ and $\mathcal{S}_1 \neq \mathcal{S}_1^*$ until $k \geq k_0$

→ Unsafe but **complete** identification