Optimization methods for ℓ_0-problems

Théo Guyard

ML MTP – December 9th, 2024

Sparse optimization

Minimize a cost with a sparse solution

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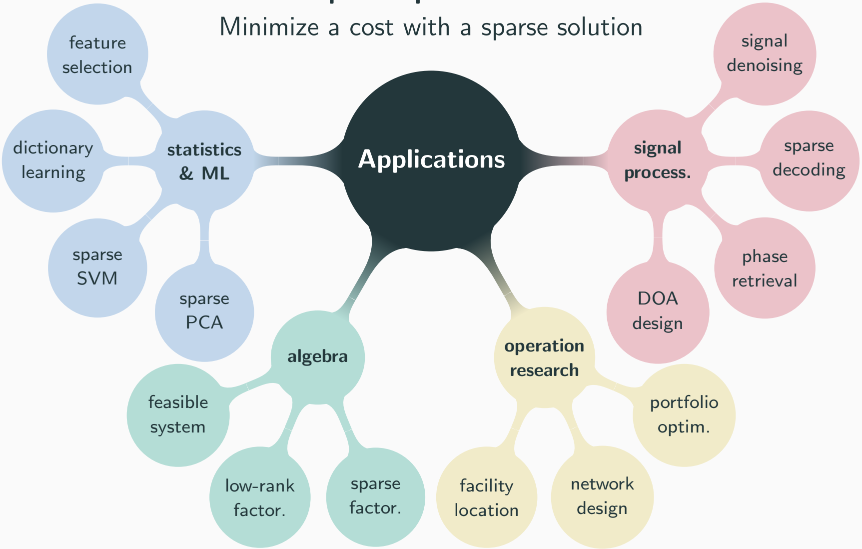
Minimize a cost with a sparse solution



A. Tillmann *et. al* (2024)

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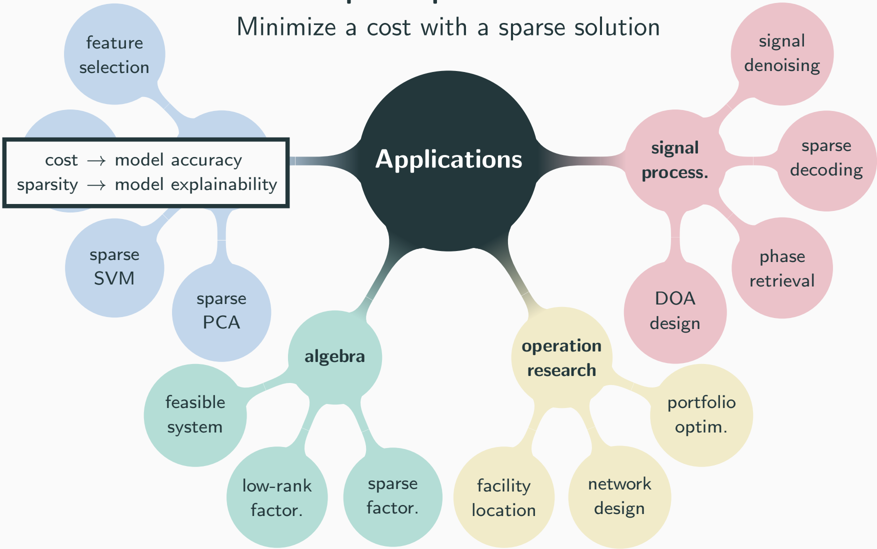

cost $\longrightarrow$ model accuracy
sparsity $\longrightarrow$ model explainability

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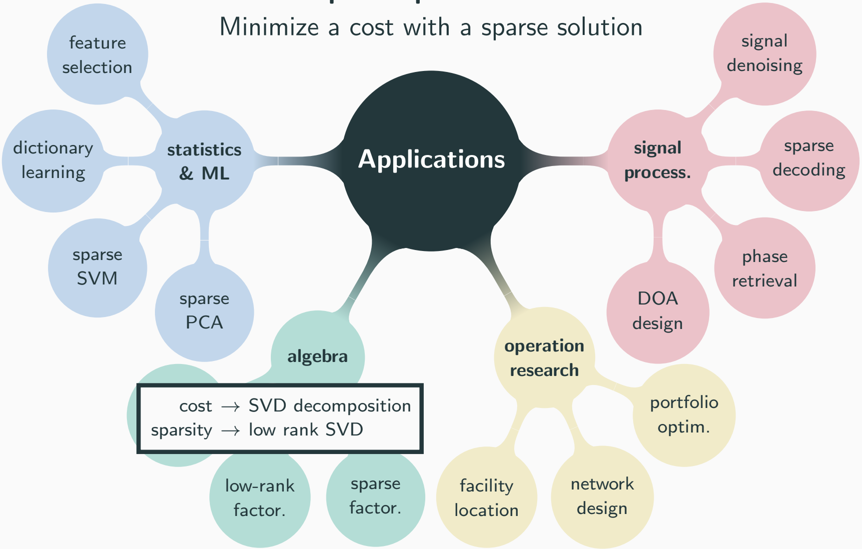

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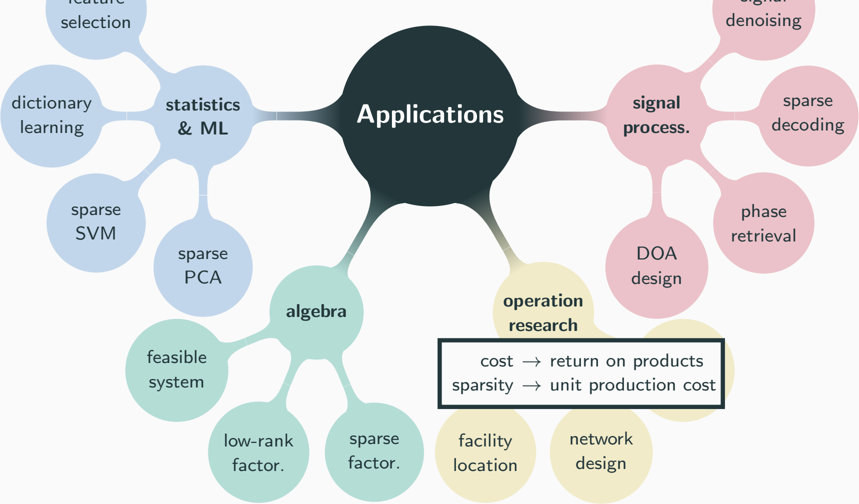

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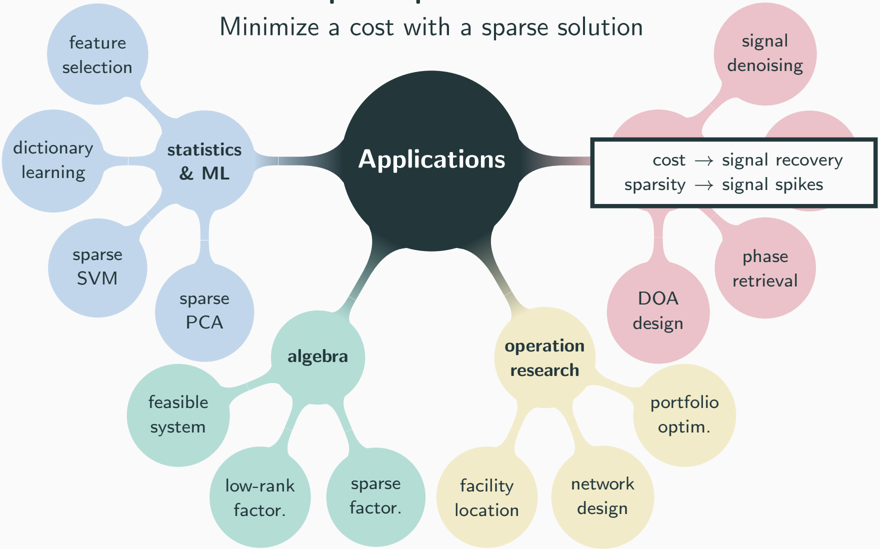

A. Tillmann *et. al* (2024)

Minimized, constrained, or regularized problem ?

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quantify cost

$f(\mathbf{x})$

thing to minimize

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$\|\mathbf{x}\|_0$

counts non-zeros

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Constrained version

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

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

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Regularized version

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

Minimized, constrained, or regularized problem ?

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Regularized version

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

$+\ h(\mathbf{x})$ separable

A bit of history

Problem

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

A bit of history

Problem

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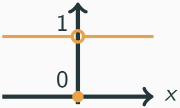
1d graph



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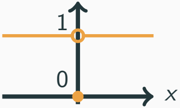

non-convex, non-diff., non-continuous, ...

A bit of history

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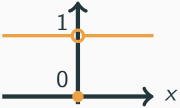
$\min_{\mathbf{x}\in\mathbf{R}^n} f(\mathbf{x}) + \lambda\|\mathbf{x}\|_0 + h(\mathbf{x})$

NP-hard to solve

1d graph



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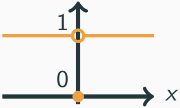

non-convex, non-diff.,
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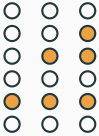
1995

Heuristics

MP, OMP, ...
S. Mallat (1993)



$\mathbf{x}^1$ $\mathbf{x}^2$ $\mathbf{x}^3$

A bit of history

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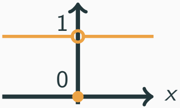

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1995 | **2000**

Heuristics
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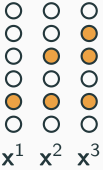
Recovery cond.
RIP, NSP, ...
E. Candes (2004)



OMP solves
ℓ_0-problem
under RIP

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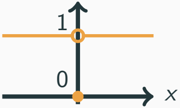

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1995 — Heuristics
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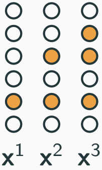
2005 — Convex approx.
Lasso, Elastic-Net, ...
R. Tibshirani (2005)



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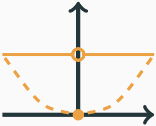

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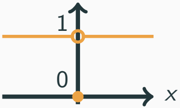

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Convex approx.
Lasso, Elastic-Net, ...
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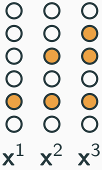
2010

Concave approx.
SCAD, MCP, ...
C. Zhang (2010)



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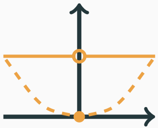

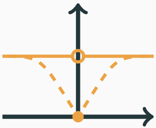

A bit of history

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NP-hard to solve

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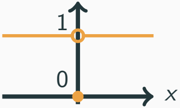
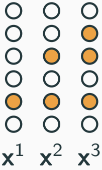


non-convex, non-diff.,
non-continuous, ...

1995	2000	2005	2010	2015
Heuristics	Recovery cond.	Convex approx.	Concave approx.	Exact methods
MP, OMP, ...	RIP, NSP, ...	Lasso, Elastic-Net, ...	SCAD, MCP, ...	MIP, BnB, ...
S. Mallat (1993)	E. Candes (2004)	R. Tibshirani (2005)	C. Zhang (2010)	D. Bertsimas (2016)



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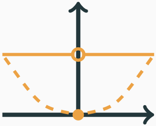

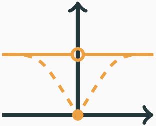

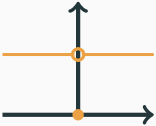

Topic of this talk

Ok, ℓ_0-problems can be of practical interest !

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🤓

What are the solution methods then ?

🤔

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1) MIP-based methods

Convenient for practitioners

Poor numerical performances

Topic of this talk

Ok, ℓ_0-problems can be of practical interest !

What are the solution methods then ?

1) MIP-based methods

Convenient for practitioners

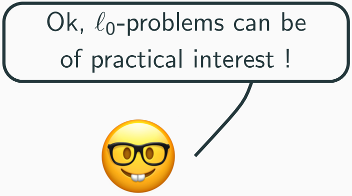
Poor numerical performances

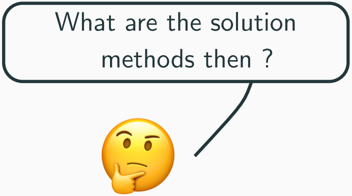
2) Specialized Branch-and-Bound

More sophisticated mechanism

Better numerical performances

Topic of this talk





1) MIP-based methods

Convenient for practitioners

Poor numerical performances

2) Specialized Branch-and-Bound

More sophisticated mechanism

Better numerical performances

High-level concepts and practical tools

Mixed-Integer Programming

MIP – Pipeline

Application

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

$\downarrow$

Problem

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

MIP – Pipeline

Application

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

$\downarrow$

Problem

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

$\downarrow$

MIP formulation

Standardized expressions

MIP – Pipeline

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

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MIP formulation

Standardized expressions

Modelling framework

Python $\rightarrow$ `cvxpy`

Julia $\rightarrow$ `JuMP`

C++ $\rightarrow$ `CMPL`

Matlab $\rightarrow$ `YALMIP`

...

MIP – Pipeline

Application

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

↓

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Problem solutions

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MIP formulation

Standardized expressions

$\downarrow$

Generic MIP solver

Gurobi, CPLEX, SCIP,
Mosek, CbC, ...

Problem solutions

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

MIP formulation

Use standardized expressions

linear, quadratic, conic, ...

Linearize ℓ_0-norm

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

$$
\begin{aligned}
x_i &= 0 \iff z_i = 0,\ \forall i \\
x_i &\neq 0 \iff z_i = 1,\ \forall i
\end{aligned}
$$

with $\mathbf{x} \in \mathbf{R}^n$ and $\mathbf{z} \in \{0,1\}^n$

MIP – Formulation

Problem

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

$\downarrow$ linearize ℓ_0-norm $\downarrow$

Linearized formulation

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

MIP formulation

Use standardized expressions

linear, quadratic, conic, ...

Linearize ℓ_0-norm

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

$$x_i = 0 \iff z_i = 0, \ \forall i$$
$$x_i \neq 0 \iff z_i = 1, \ \forall i$$

with $\mathbf{x} \in \mathbf{R}^n$ and $\mathbf{z} \in \{0,1\}^n$

MIP – Formulation

Problem

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

linearize ℓ_0-norm

Linearized formulation

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

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with $\mathbf{x} \in \mathbf{R}^n$ and $\mathbf{z} \in \{0,1\}^n$

Avoid logical constraint

$$h_{\mathrm{mip}}(\mathbf{x},\mathbf{z}) = \begin{cases} h(\mathbf{x}) & \text{if } x_i = 0 \iff z_i = 0 \\ +\infty & \text{otherwise} \end{cases}$$

MIP – Formulation

Problem

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linearize ℓ_0-norm

Linearized formulation

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avoid logical cstr.

MIP formulation

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

MIP formulation

Use standardized expressions

linear, quadratic, conic, ...

Linearize ℓ_0-norm

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

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Sparse regression

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

Sparse regression

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

$\downarrow$

Optimization problem

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

- $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{y} - \mathbf{Ax}\|_2^2$
- $h(\mathbf{x}) = \mathrm{Ind}(-M \leq \mathbf{x} \leq M)$

Sparse regression

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

$$\downarrow$$

Optimization problem

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

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MIP – Hands-on with `cvxpy`

Sparse regression

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

$\downarrow$

Optimization problem

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

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$\downarrow$

MIP formulation

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```
$ pip install cvxpy
```

MIP – Hands-on with cvxpy

Sparse regression

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

$\downarrow$

Optimization problem

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

- $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathrm{Ind}(-M \leq \mathbf{x} \leq M)$

$\downarrow$

MIP formulation

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

```
$ pip install cvxpy
```

```python
import cvxpy as cp

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

MIP – Hands-on with cvxpy

Sparse regression

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

$\downarrow$

Optimization problem

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

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```
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)
```

MIP – Hands-on with cvxpy

Sparse regression

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

$\downarrow$

Optimization problem

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

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```
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# 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
obj = cp.Minimize(
    cp.sum_squares(A @ x - y) +
    0.01 * cp.sum(z)
)
cst = [-5.0 * z <= x, x <= 5.0 * z]
```

MIP – Hands-on with cvxpy

Sparse regression

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

$\downarrow$

Optimization problem

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

- $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{y} - \mathbf{Ax}\|_2^2$
- $h(\mathbf{x}) = \mathrm{Ind}(-M \leq \mathbf{x} \leq M)$

$\downarrow$

MIP formulation

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

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obj = cp.Minimize(
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    0.01 * cp.sum(z)
)
cst = [-5.0 * z <= x, x <= 5.0 * z]

# Solve the problem using Gurobi
problem = cp.Problem(obj, cst)
problem.solve(solver=cp.GUROBI)
```

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

2) Establish MIP formulation

3) Use generic MIP solvers

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

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3) Use generic MIP solvers

Pros

✓ Rich MIP literature

✓ Black-box solvers

✓ Convenient for practitioners

MIP – Let's sum up

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

Pipeline

1) Introduce binary variable

2) Establish MIP formulation

3) Use generic MIP solvers

Pros

✓ Rich MIP literature

✓ Black-box solvers

✓ Convenient for practitioners

Cons

✗ Mostly commercial solvers

✗ Unable to exploit structure

✗ Performance issues

Branch-and-Bound Algorithms

BnB – Pipeline

Application

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

$\downarrow$

Problem

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

BnB – Pipeline

Application

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

$\downarrow$

Problem

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

$\downarrow$

Design BnB solver

Specialized mechanisms

BnB – Pipeline

Application

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

$\downarrow$

Problem

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

$\downarrow$

Design BnB solver

Specialized mechanisms

$\downarrow$

Problem solutions

BnB – Pipeline

Application

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

↓

Problem

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

↓

~~**Design BnB solver**~~

~~Specialized mechanisms~~

↓

Problem solutions

Existing BnB solver

`sbnb` → G. Samain *et al.* (2020)

`l0bnb` → H. Hazimeh *et al.* (2021)

`el0ps` → T. Guyard *et al.* (2024)

BnB – Pipeline

Application

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

↓

Problem

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

↓

~~**Design BnB solver**~~

~~Specialized mechanisms~~

↓

Problem solutions

Existing BnB solver

`sbnb` → G. Samain *et al.* (2020)

`l0bnb` → H. Hazimeh *et al.* (2021)

`el0ps` → T. Guyard *et al.* (2024)

Why using `el0ps` ?

Is is fast and flexible !

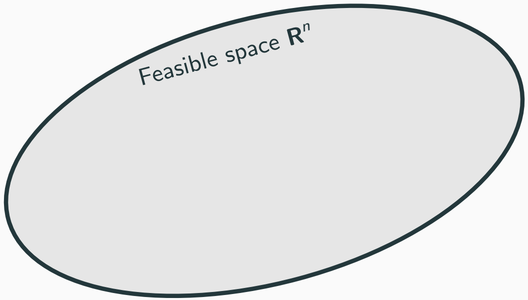
😎

BnB – Algorithmic principle

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

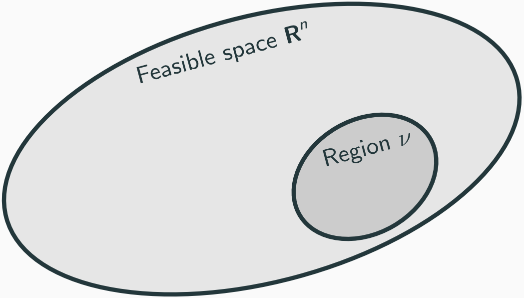
BnB – Algorithmic principle

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



BnB – Algorithmic principle

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



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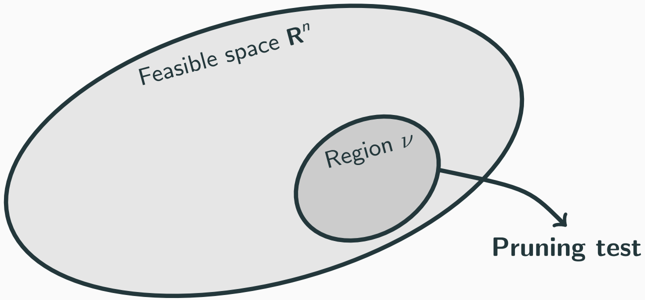
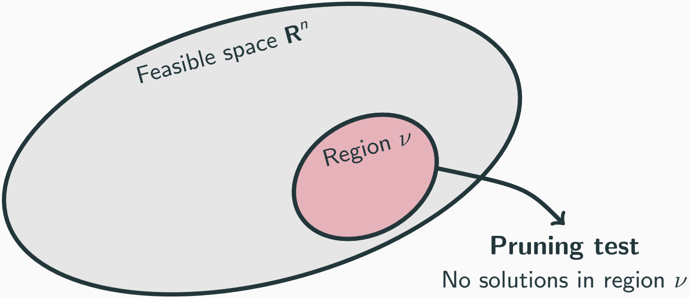


BnB – Algorithmic principle

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



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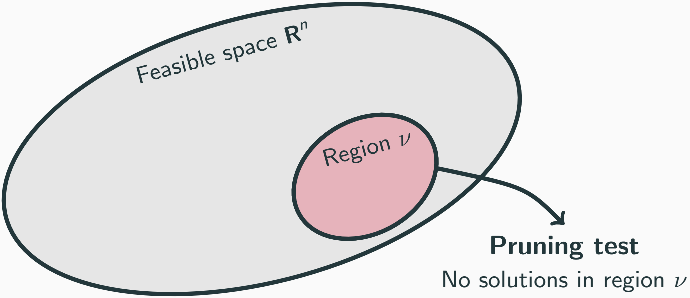


Branching step – Region design and exploration
Bounding step – Pruning test evaluation

BnB – Branching step

Problem

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

BnB – Branching step

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

BnB – Branching step

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

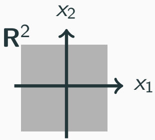
BnB – Branching step

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

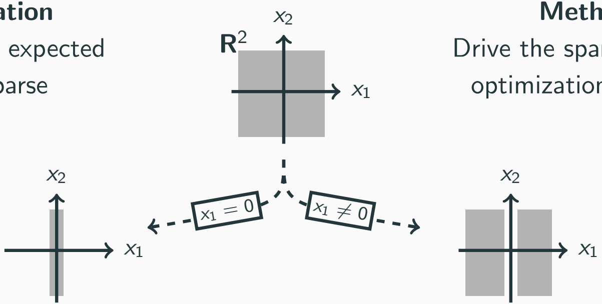
BnB – Branching step

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



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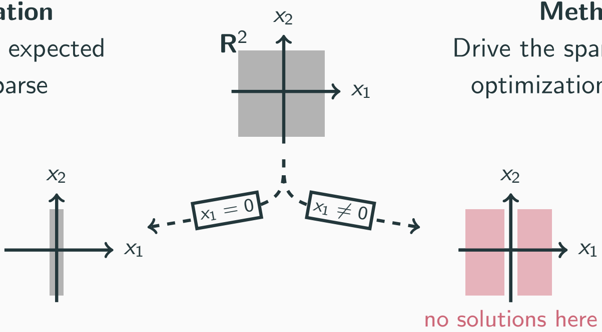

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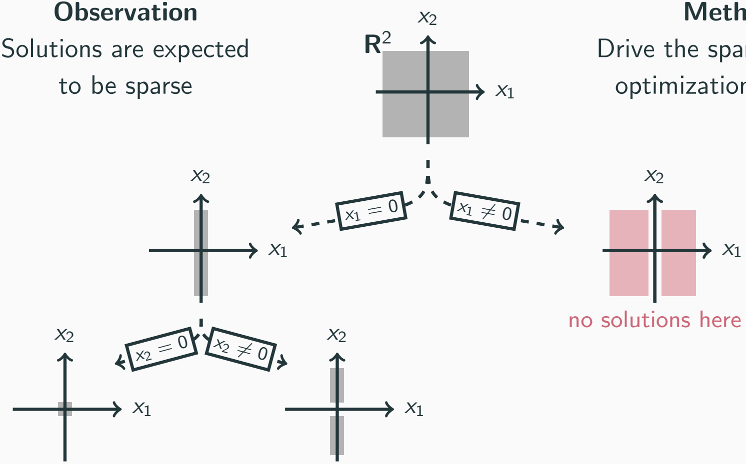

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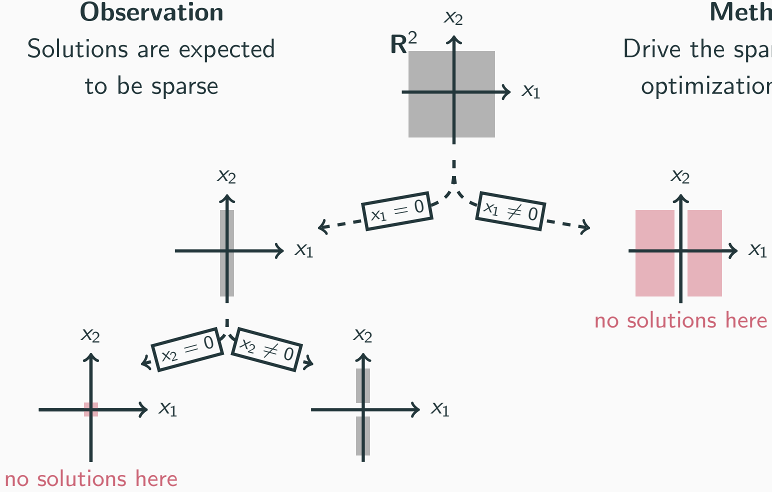

Problem

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

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Solutions are expected to be sparse

Method

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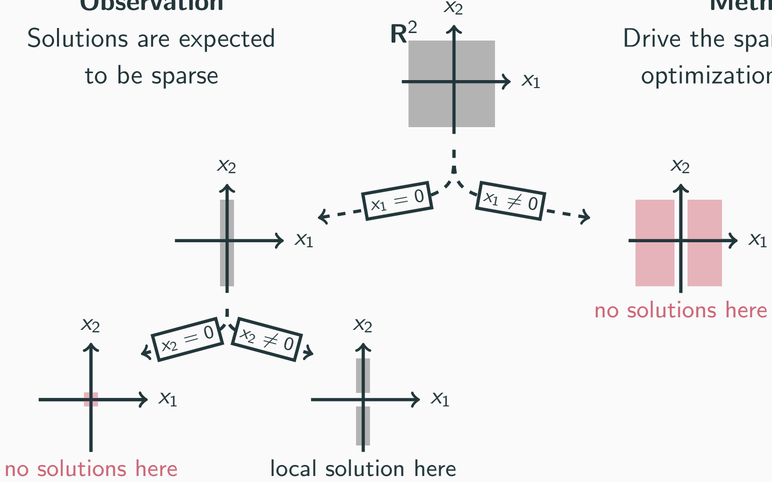


BnB – Branching step

Problem

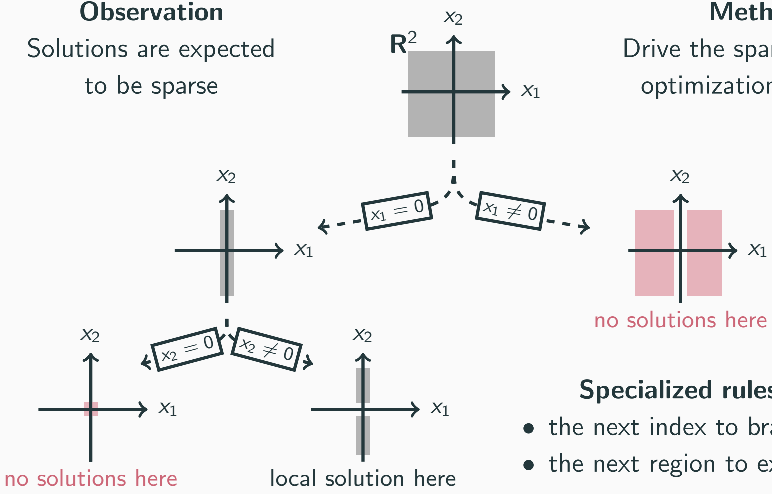
$\min_{\mathbf{x}\in\mathbf{R}^n} f(\mathbf{x}) + \lambda\|\mathbf{x}\|_0 + h(\mathbf{x})$

Observation

Solutions are expected to be sparse

Method

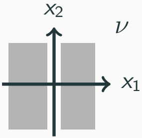
Drive the sparsity of the optimization variable



Specialized rules for

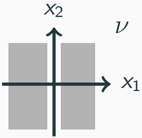
- the next index to branch on
- the next region to explore

BnB – Bounding step



Does region ν contains optimal solutions ?

BnB – Bounding step

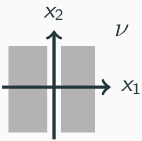


Does region ν contains optimal solutions ?

Problem

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

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

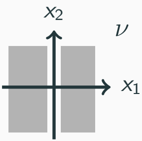
$p^\star = \min_{\mathbf{x}\in\mathbf{R}^n} f(\mathbf{x}) + \lambda\|\mathbf{x}\|_0 + h(\mathbf{x})$

$\downarrow$ restrict to ν

Restriction to region ν

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

BnB – Bounding step



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Problem

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

$\downarrow$ restrict to ν

Restriction to region ν

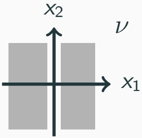
$$p^\nu = \min_{\mathbf{x}\in\nu} f(\mathbf{x}) + \lambda\|\mathbf{x}\|_0 + h(\mathbf{x})$$

$\downarrow$ compare

Pruning test

$$p^\nu > p^\star$$

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

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

restrict to ν

Restriction to region ν

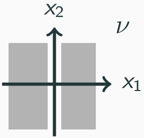
$p^\nu = \min_{\mathbf{x} \in \nu} \; f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$

compare

Pruning test

$p^\nu > p^\star$ $\longrightarrow$ prune ν

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

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

restrict to ν

Restriction to region ν

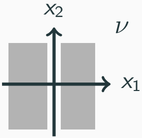
$p^\nu = \min_{\mathbf{x}\in\nu} \; f(\mathbf{x}) + \lambda\|\mathbf{x}\|_0 + h(\mathbf{x})$

compare

Pruning test

$p^\nu_{\mathrm{lb}} > p^\star_{\mathrm{ub}}$ $\longrightarrow$ prune ν

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

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

↓ restrict to ν

Restriction to region ν

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

↓ compare

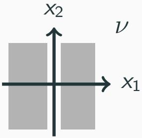
Pruning test

$p^\nu_{\mathrm{lb}} > p^\star_{\mathrm{ub}}$ $\longrightarrow$ prune ν

Easy task

Compute an upper bound on $p^\star$

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

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

restrict to ν

Restriction to region ν

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

compare

Pruning test

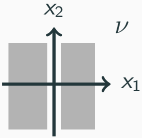
$p^\nu_{\text{lb}} > p^\star_{\text{ub}}$ $\longrightarrow$ prune ν

Easy task

$\boxed{\text{Compute an upper bound on } p^\star}$

Construct and evaluate
a feasible vector in each
region explored to refine $p^\star_{\text{ub}}$

BnB – Bounding step



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Restriction to region ν

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

$\downarrow$ compare

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Construct and evaluate
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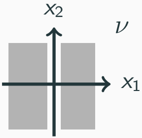
Main challenge

$\boxed{\text{Compute a lower bound on } p^\nu}$

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

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

restrict to ν

Restriction to region ν

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

compare

Pruning test

$p^\nu_{\mathrm{lb}} > p^\star_{\mathrm{ub}}$ $\longrightarrow$ prune ν

Easy task

Compute an upper bound on $p^\star$

Construct and evaluate
a feasible vector in each
region explored to refine $p^\star_{\mathrm{ub}}$

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

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

seek tight/tractable lower bound on p^ν

$\downarrow$ reformulation

Restriction to region ν

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

with g^ν proper and closed

BnB – Building relaxations

Restriction to region ν

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

seek tight/tractable lower bound on p^ν

$\downarrow$ reformulation

Restriction to region ν

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

with g^ν proper and closed

$\downarrow$ $g^\nu_{\text{lb}} \leq g^\nu$, g^ν_{lb} convex

Relaxation for region ν

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

set g^ν_{lb} set as the convex envelope of g^ν

BnB – The full picture

Problem

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

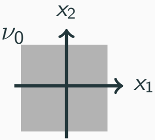
BnB – The full picture

Problem

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

Best upper bound

$p^\star_{\mathrm{ub}} = +\infty$



BnB – The full picture

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Best upper bound

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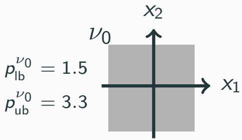


BnB – The full picture

Problem

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

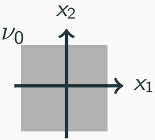
Best upper bound

$\cancel{p^\star_{\text{ub}} = +\infty}$

$p^\star_{\text{ub}} = 3.3$

$p^{\nu_0}_{\text{lb}} = 1.5$

$p^{\nu_0}_{\text{ub}} = 3.3$



BnB – The full picture

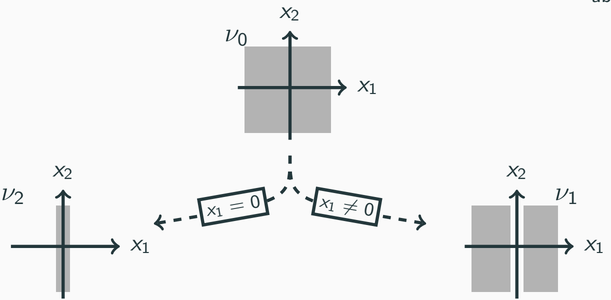
Problem

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

Best upper bound

$\cancel{p^\star_{\mathrm{ub}} = +\infty}$

$p^\star_{\mathrm{ub}} = 3.3$



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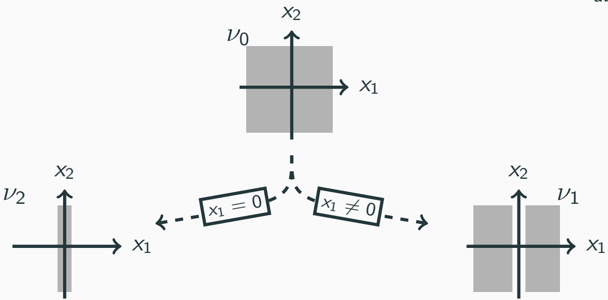

$p^{\nu_1}_{\mathrm{lb}} = 4.5$

BnB – The full picture

Problem

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

Best upper bound

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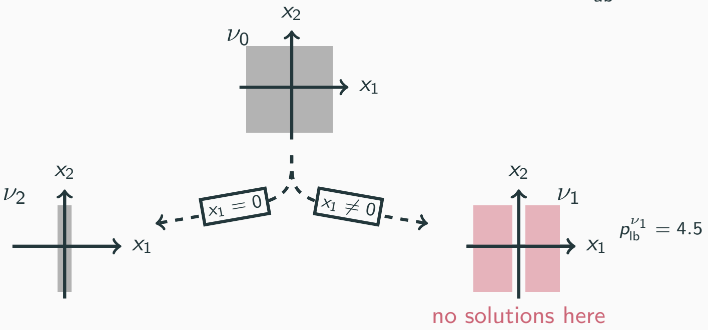

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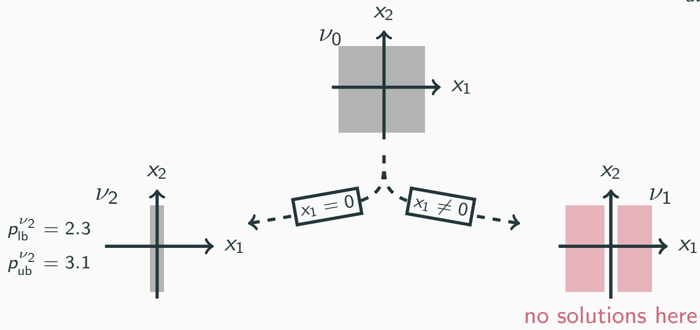

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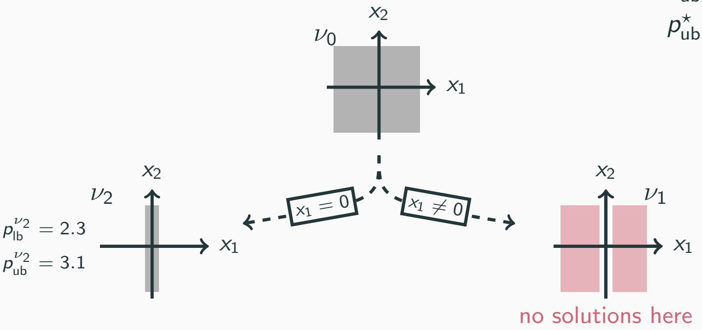
$p^\star_{\text{ub}} = 3.1$



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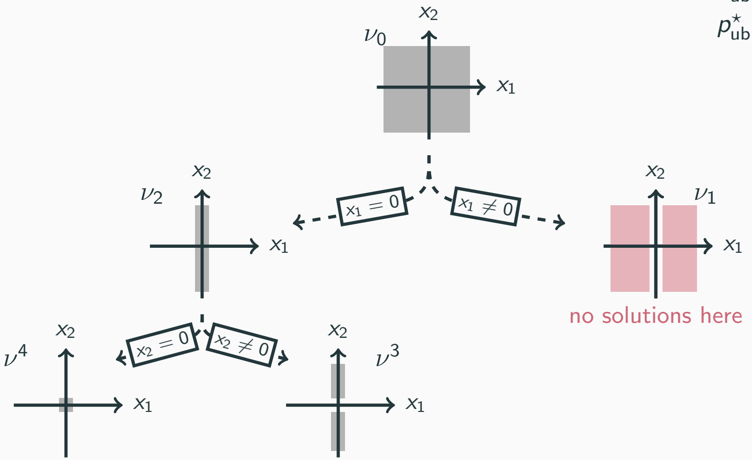

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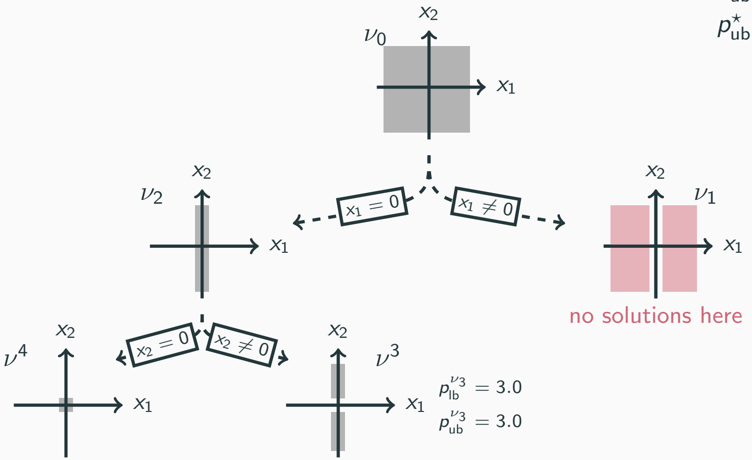

$p^{\nu_3}_{\text{lb}} = 3.0$

$p^{\nu_3}_{\text{ub}} = 3.0$

BnB – The full picture

Problem

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

Best upper bound

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$\cancel{p^\star_{\text{ub}} = 3.1}$

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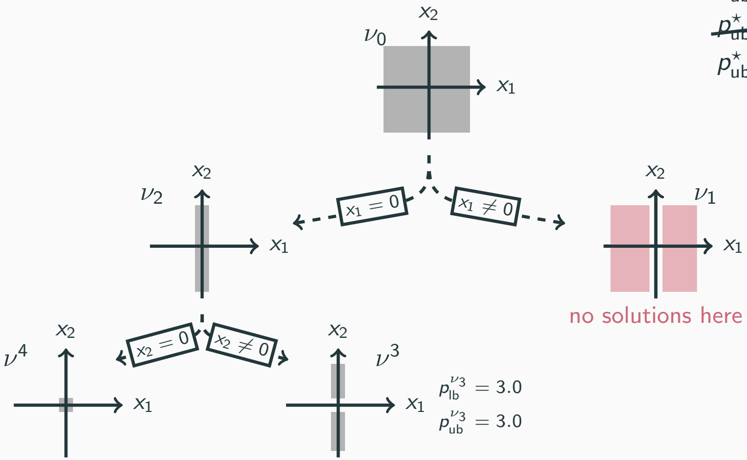

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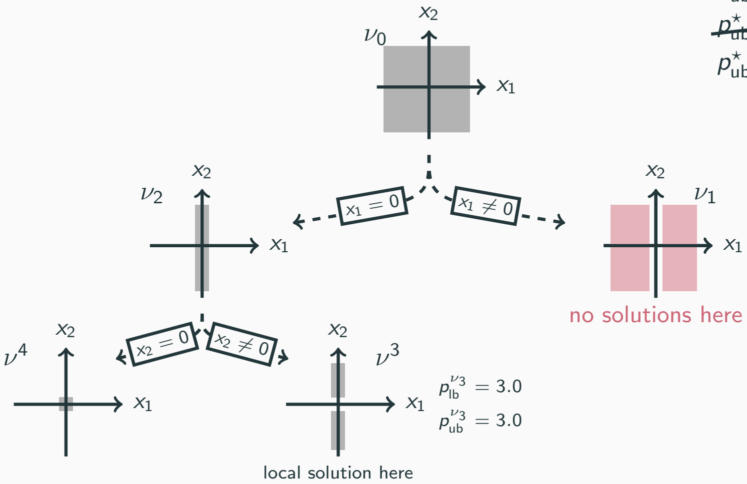

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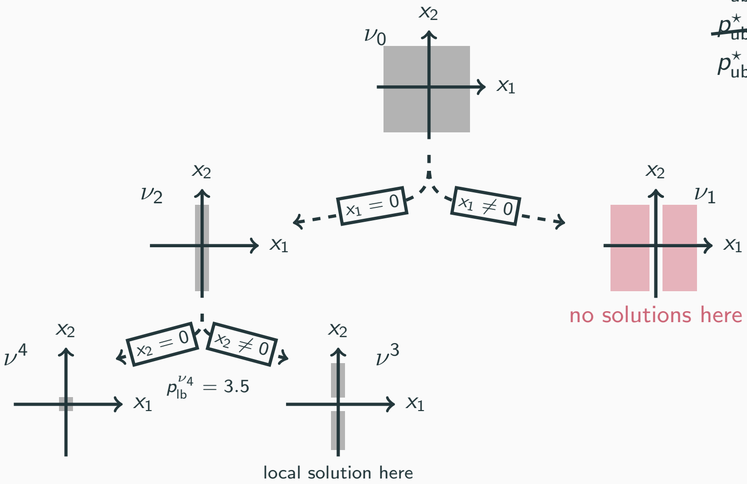

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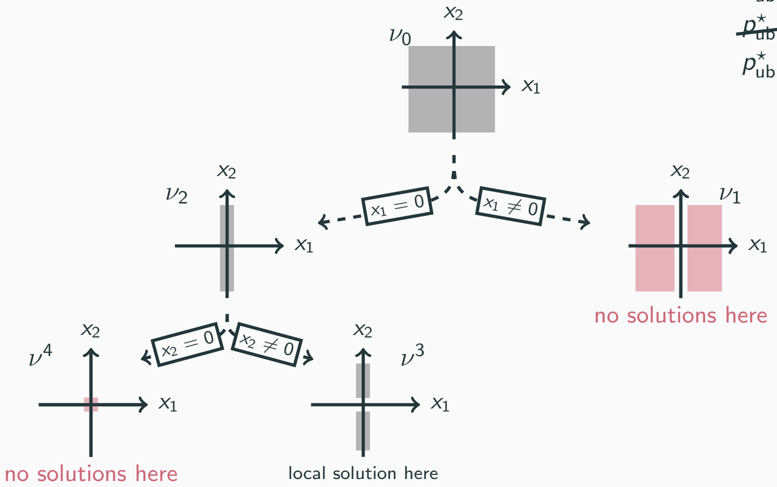

BnB – The secrete sauce

Solve time

region processing time $\times$ number of regions processed

BnB – The secrete sauce

Solve time

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

Relaxation for region ν

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

BnB – The secrete sauce

Solve time

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

Relaxation for region ν

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

g_{lb}^{ν} is proper, closed, convex, separable, and non-diff. at $\mathbf{x} = \mathbf{0}$

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This is a convex sparse optimization problem !

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$\rightarrow$ first-order methods

proximal gradient, coordinate descent, ...

$\rightarrow$ acceleration strategies

working set, screening tests, ...

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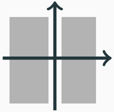

processing region ...

BnB – The secrete sauce

Solve time

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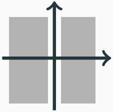

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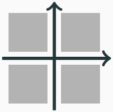

perform degraded but low-cost pruning test

Solve time

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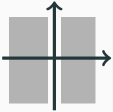
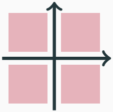


processing region ...



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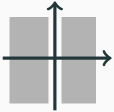

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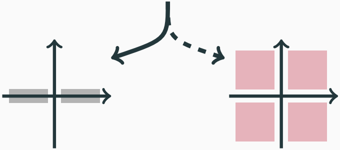

continue processing

perform degraded but low-cost pruning test

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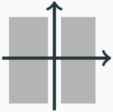
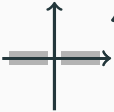
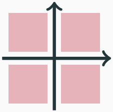


processing region ...



continue processing

bypass region



perform degraded but low-cost pruning test

Sparse regression

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

Sparse regression

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

$\downarrow$

Optimization problem

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

- $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathrm{Ind}(-M \leq \mathbf{x} \leq M)$

```
$ pip install el0ps
```

Sparse regression

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

$\downarrow$

Optimization problem

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

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

BnB – Hands-on with `el0ps`

```
$ pip install el0ps
```

Sparse regression

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

$\downarrow$

Optimization problem

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

- $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{y} - \mathbf{Ax}\|_2^2$
- $h(\mathbf{x}) = \mathrm{Ind}(-M \leq \mathbf{x} \leq M)$

```python
from el0ps.datafits import Leastsquares
from el0ps.penalties import Bigm
from el0ps.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 regression

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

$$\downarrow$$

Optimization problem

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

- $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2$
- $h(\mathbf{x}) = \mathrm{Ind}(-M \leq \mathbf{x} \leq M)$

```
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from el0ps.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 el0ps' solver
solver = BnbSolver()
solver.solve(f, h, lmbd=0.01)
```

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 specialized BnB

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 specialized BnB

1b) Use an existing BnB solver

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Pros

✓ Numerical efficiency

✓ Open-source softwares

✓ Convenient for practitioners

BnB – Let's sum up

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Pipeline

1a) Implement a specialized BnB

1b) Use an existing BnB solver

2) Solve the problem

Pros

✓ Numerical efficiency

✓ Open-source softwares

✓ Convenient for practitioners

Cons

✗ Assumptions on f/h

✗ f/h proper, closed, convex

✗ f smooth, h coercive

Conclusion

A community with a bunch of people

Non-exhaustive list

A community with a bunch of people

Non-exhaustive list

MIT

D. Bertsimas, R. Mazmuder, ...

Optimization tools for ℓ_0-problems

A community with a bunch of people

Non-exhaustive list

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Google Deep Mind
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MIP-based heuristics

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Convex-based acceleration

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M. Carlsson, C. Olsson...
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Healthcare applications

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

Centrale Nantes / ENSTA Bretagne
S. Bourguignon, J. Ninin, ...
BnB with quadratic loss

Inria / CentraleSupélec
C. Herzet, C. Elvira, A. Arslan, ...
Generic and efficient BnB

IRIT / I3S
E. Soubies, L. Blanc-Féraud, ...
Convex-concave relaxation

Take-home messages

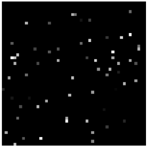
- Although NP-hard, ℓ_0-problems are of practical interest
- There exists methods to tackle them
  - MIP-based formulation and generic solvers
  - BnB algorithms with specialized steps
  - Structure-exploitation is key
- It's an active research area
  - Theoretical and methodological developments still needed
  - Need to reach the applicative world

Question time !

🤓

Compressed sensing

Sparse signal
$\mathbf{x} \in \mathbf{R}^n$



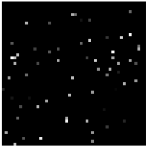
n pixels

Compressed sensing

Linear compression

Sparse signal

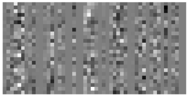
$\mathbf{x} \in \mathbf{R}^n$



n pixels

Compressed signal

$\mathbf{y} = \mathbf{A}\mathbf{x} \in \mathbf{R}^m$

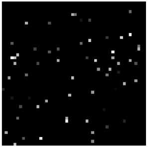


m pixels, $m \ll n$

Compressed sensing

Sparse signal

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



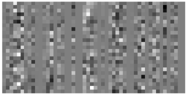
n pixels

Linear compression

Recover $\mathbf{x}$ from $\mathbf{A}$ and $\mathbf{y}$

Compressed signal

$\mathbf{y} = \mathbf{A}\mathbf{x} \in \mathbf{R}^m$



m pixels, $m \ll n$

Compressed sensing

Sparse signal

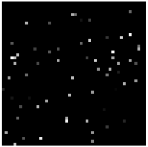
$\mathbf{x} \in \mathbf{R}^n$

Linear compression

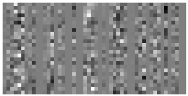
Recover $\mathbf{x}$ from $\mathbf{A}$ and $\mathbf{y}$

Compressed signal

$\mathbf{y} = \mathbf{A}\mathbf{x} \in \mathbf{R}^m$



n pixels



m pixels, $m \ll n$

Goal

Find $\mathbf{x}$ such that $\mathbf{y} = \mathbf{A}\mathbf{x}$

Compressed sensing

Sparse signal

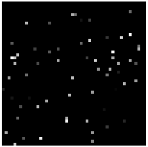
$\mathbf{x} \in \mathbf{R}^n$

Linear compression

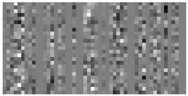
Recover $\mathbf{x}$ from $\mathbf{A}$ and $\mathbf{y}$

Compressed signal

$\mathbf{y} = \mathbf{A}\mathbf{x} \in \mathbf{R}^m$



n pixels



m pixels, $m \ll n$

Goal

Find $\mathbf{x}$ such that $\mathbf{y} = \mathbf{A}\mathbf{x}$

no unique solution

Goal

Find $\mathbf{x}$ sparse such that $\mathbf{y} = \mathbf{A}\mathbf{x}$

Feature selection

	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	$a_{3,1}$	$\boxed{\mathbf{A} \in \mathbf{R}^{m \times n}}$	...	$a_{3,n}$	$\boxed{\mathbf{y} \in \mathbf{R}^m}$
...	...	...	...	...	...
Sample m	$a_{m,1}$	$a_{m,2}$	...	$a_{m,n}$	y_m

Feature selection

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

Features $\mathbf{A} \in \mathbf{R}^{m \times n}$ $\xleftrightarrow[\text{weights } \mathbf{x} \in \mathbf{R}^n]{}$ Target $\mathbf{y} = \phi(\mathbf{A}\mathbf{x})$

Feature selection

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

Features $\mathbf{A} \in \mathbf{R}^{m \times n} \xleftrightarrow[\text{weights } \mathbf{x} \in \mathbf{R}^n]{}$ Target $\mathbf{y} = \phi(\mathbf{Ax})$

Model accuracy

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

Model explainability

Use few features

Feature selection

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

Features $\mathbf{A} \in \mathbf{R}^{m \times n}$ $\xleftrightarrow[\text{weights } \mathbf{x} \in \mathbf{R}^n]{}$ Target $\mathbf{y} = \phi(\mathbf{A}\mathbf{x})$

Model accuracy

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

$\downarrow$

Model explainability

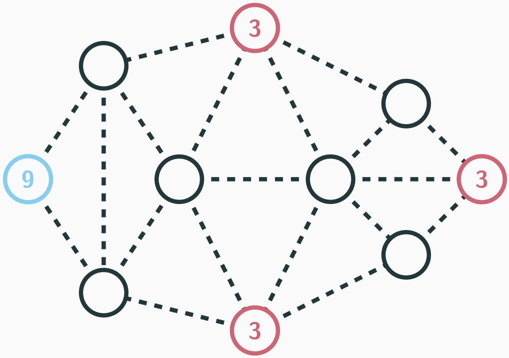
Use few features

$\downarrow$

Goal

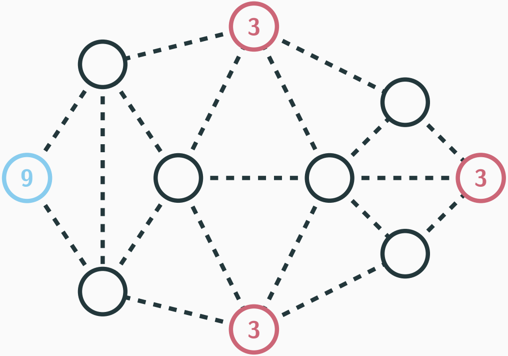
Find $\mathbf{x}$ sparse such that $\mathcal{L}_\phi(\mathbf{A}\mathbf{x}, \mathbf{y})$ is small

Network design



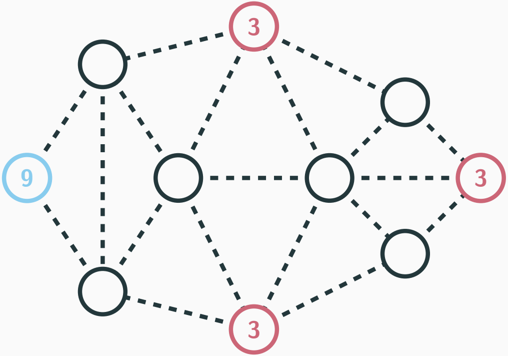
Which edges to build to transport products from source to sink nodes ?

Network design



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

Network design

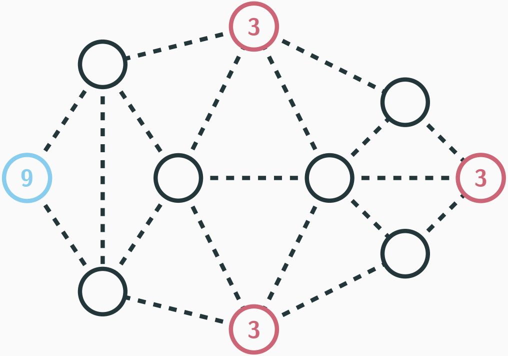


Which edges to build to transport products from source to sink nodes ?

construct edge $i \in I$ if $x_i > 0$

pay construction cost c

Network design



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

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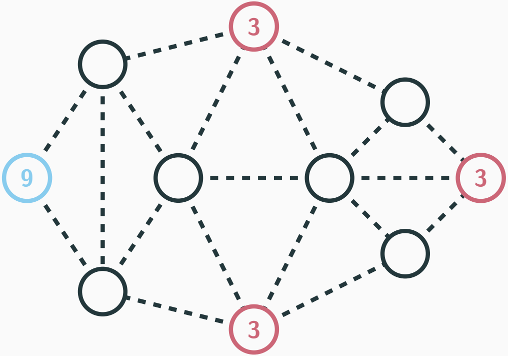
Question

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 ?

Find $\mathbf{x} \in \mathbf{R}^{\mathrm{card}(I)}$ sparse

such that $\mathcal{Q}(\mathbf{x}) = 0$

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

Balancing solution quality and problem hardness

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

Colony	AADK	AAPA	ABFA	ABH	...	ZUR	**B2 prod.**
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...	...	...	...	...	...	...	...
#71	6.85	8.27	7.98	8.04	...	6.65	**-7.58**

$\underbrace{\hspace{6em}}_{\text{4,088 genes}}$