

# Optimization methods for $\ell_0$ -problems

Théo Guyard

CIRRELT, Montréal, Canada – March 6th, 2025

# Sparse optimization

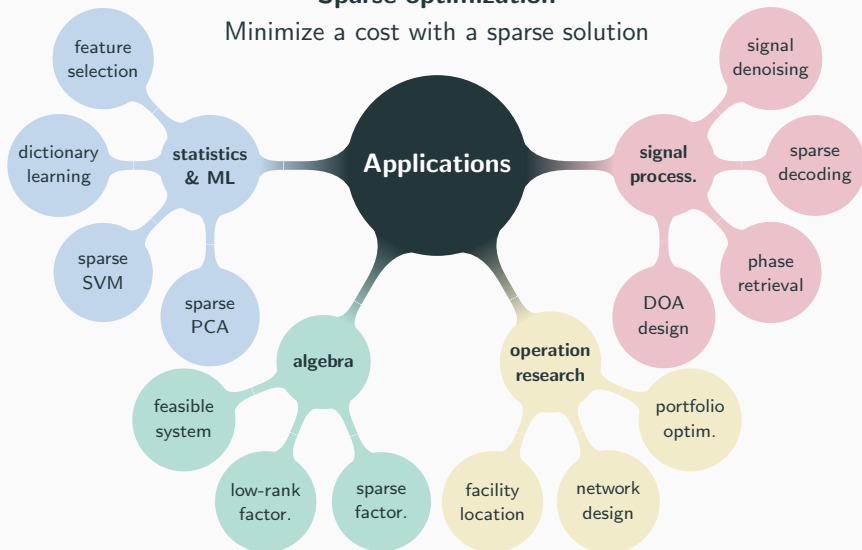
## Sparse optimization

Minimize a cost with a sparse solution

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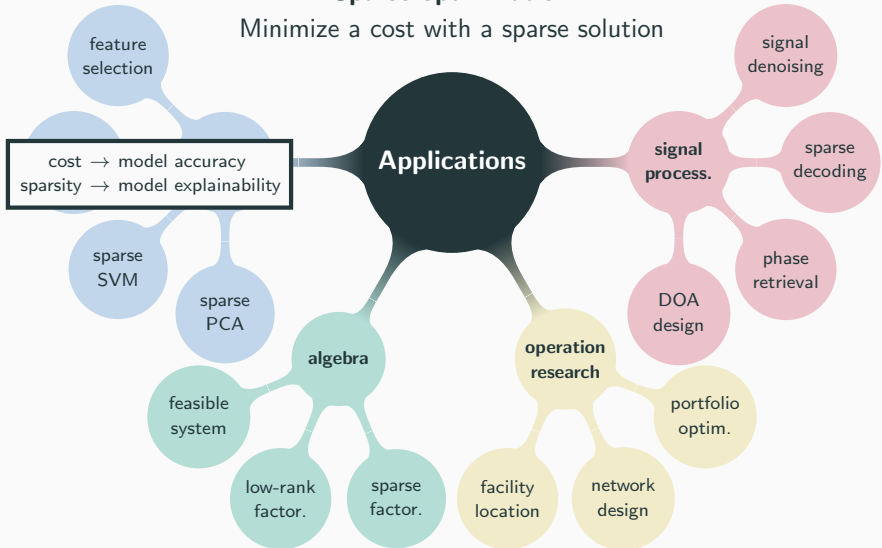
Minimize a cost with a sparse solution



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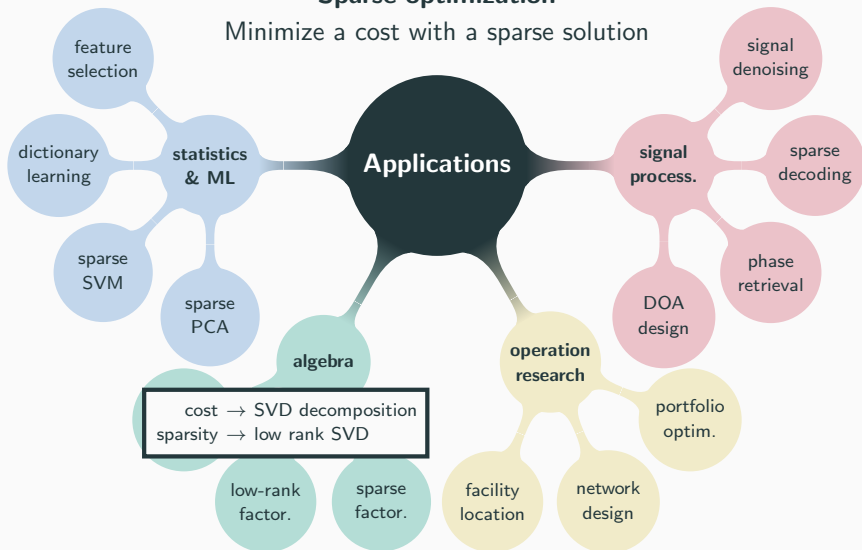
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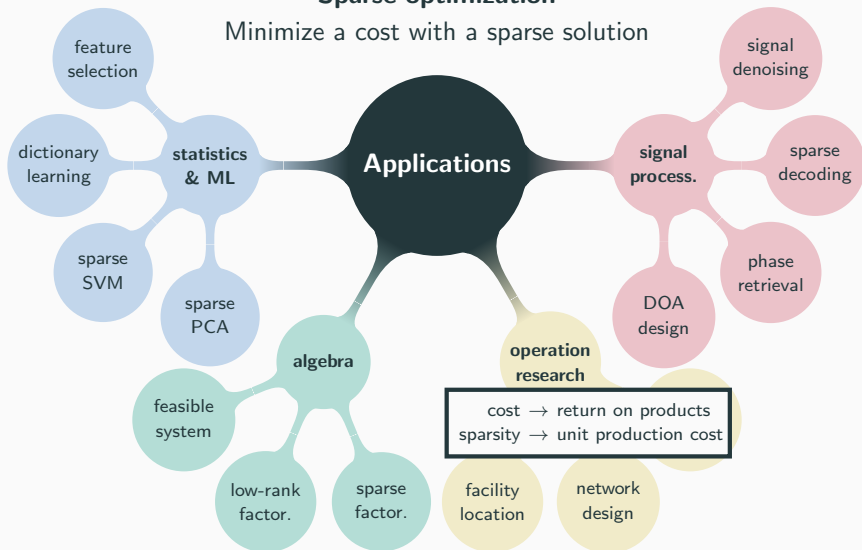
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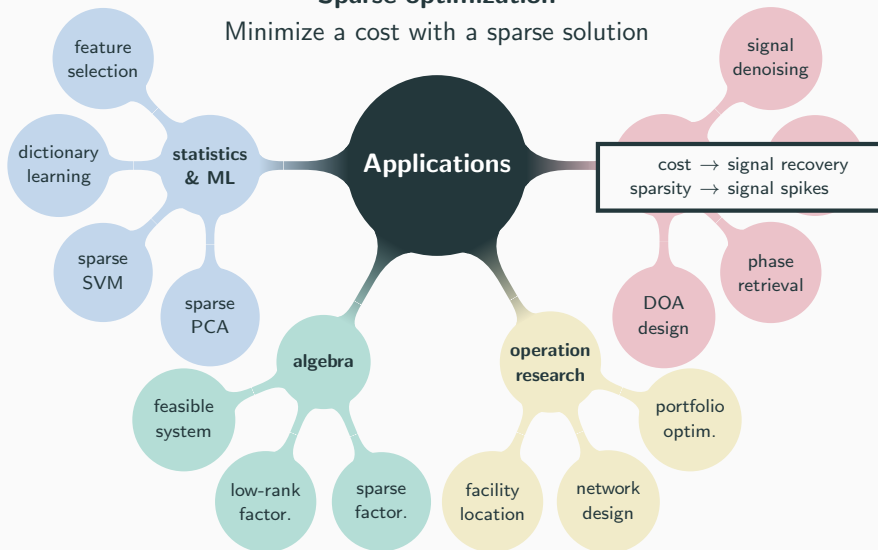
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# Minimized, constrained, or regularized problem ?

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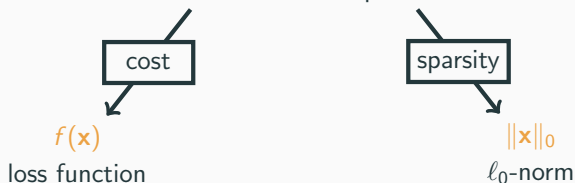
$f(\mathbf{x})$

loss function

# Minimized, constrained, or regularized problem ?

## Sparse optimization

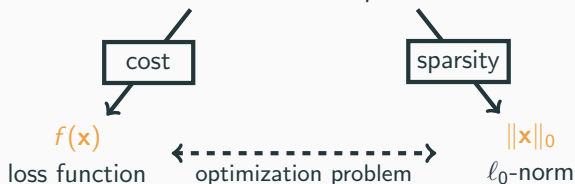
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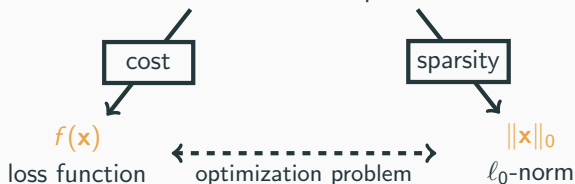
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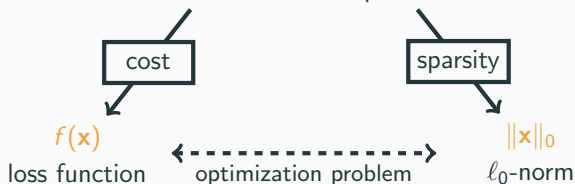
## Constrained problem

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

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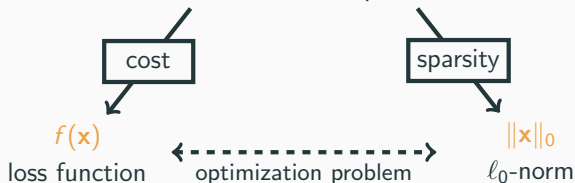
### Minimized problem

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

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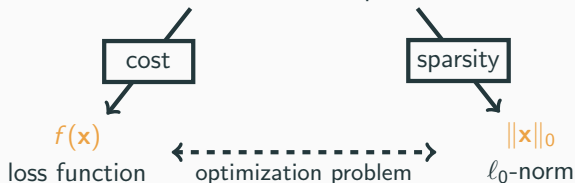
### Regularized problem

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

# Minimized, constrained, or regularized problem ?

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### Regularized problem

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

### Problem

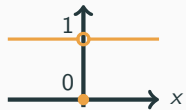
$$\min_{\mathbf{x} \in \mathbf{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$



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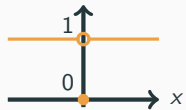
$\ell_0$ -norm in 1d



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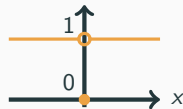
non-convex, non-smooth,  
non-continuous, ...

## Problem

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

NP-hard to solve

$\ell_0$ -norm in 1d



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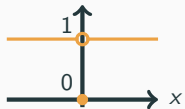
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1995

Heuristics

MP, OMP, ...

S. Mallat (1993)



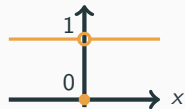
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Recovery cond.

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

Heuristics solve  
 $\ell_0$ -problem  
under some  
(strong)  
conditions

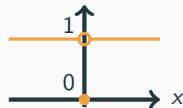
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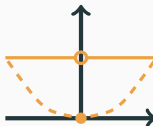
Convex approx.

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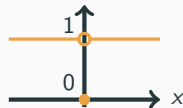
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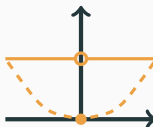
**2010**

Concave approx.

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



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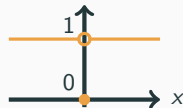
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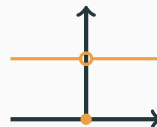
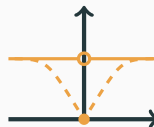
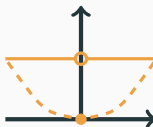
**2015**

Exact methods

MIP, BnB, ...  
D. Bertsimas (2016)



Heuristics solve  
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# Topic of this talk

Ok,  $\ell_0$ -problems can  
be addressed exactly!



(you)

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What are the solution  
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(also you if you're an optim. nerd)

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## 1) MIP-based methods

Based on off-the-shelf solvers

Poor numerical performances

# Topic of this talk

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## 1) MIP-based methods

Based on off-the-shelf solvers

Poor numerical performances

## 2) Specialized Branch-and-Bound

Tailored solution method

Better numerical performances

# Mixed-Integer Programming

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## Application

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



## Problem

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

# MIP – Pipeline

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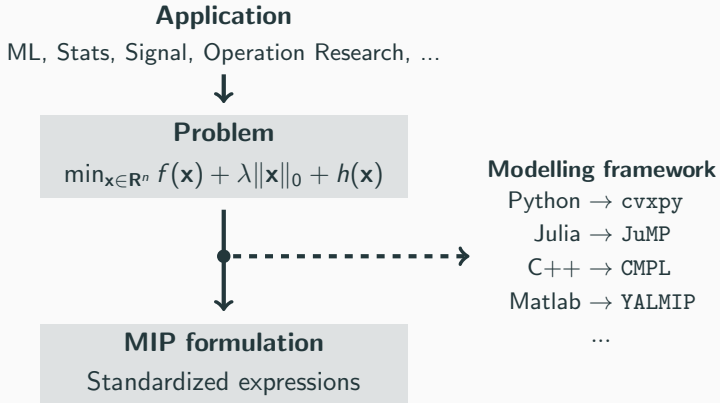
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## MIP formulation

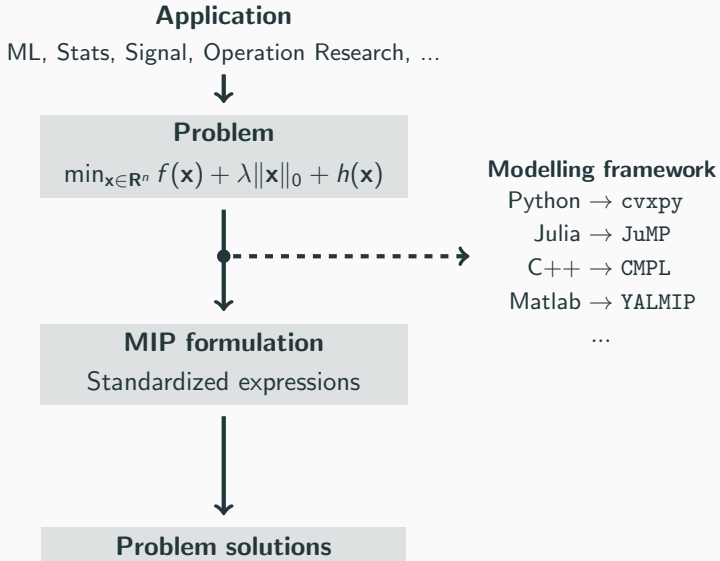
Standardized expressions

# MIP – Pipeline

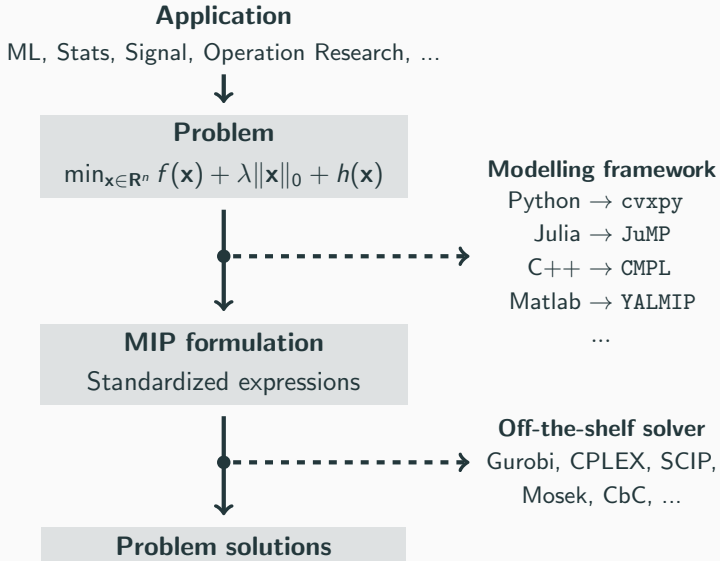




# MIP – Pipeline



# MIP – Pipeline



# 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, ...

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## MIP formulation

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## Linearize the $\ell_0$ -norm

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

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

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

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

# MIP – Formulation

## Problem

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

linearize the  $\ell_0$ -norm

## Linearized formulation

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

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## Avoid logical constraint

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

# MIP – Formulation

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avoid logical cstr.

## MIP formulation

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

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[XXX]



## Problem

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

## Pipeline

- 1) Introduce binary variable
- 2) Establish MIP formulation
- 3) Use generic MIP solvers

# MIP – Let's sum up

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- ✓ Rich MIP literature
- ✓ Black-box solvers
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## Cons

- ✗ Mostly commercial solvers
- ✗  $h$  as big-M or  $\ell_2$ -norm
- ✗ Performance issues

# Branch-and-Bound Algorithms

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## Application

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



## Problem

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

# BnB – Pipeline

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



## Problem

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



## Implement BnB solver

Specialized mechanisms

# BnB – Pipeline

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## Problem solutions

# BnB – Pipeline

**Application**  
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**Problem**

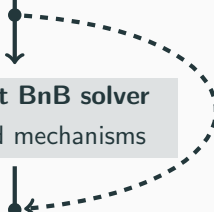
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**Implement BnB solver**  
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**Problem solutions**



## Existing BnB solver

sbnb → G. Samain *et al.* (2020)  
10bnb → H. Hazimeh *et al.* (2021)  
el0ps → T. Guyard *et al.* (2024)



# BnB – Pipeline

**Application**  
ML, Stats, Signal, Operation Research, ...



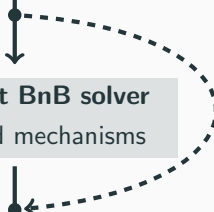
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**Implement BnB solver**  
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**Problem solutions**



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## Why using el0ps?

Is is free, fast and flexible!

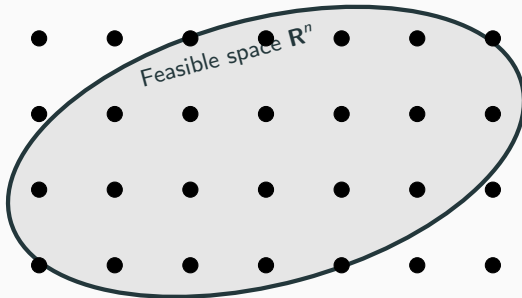


## BnB – Algorithmic principle

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

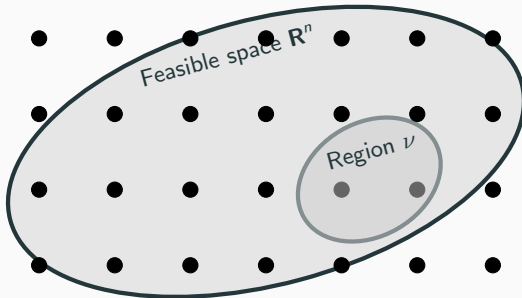
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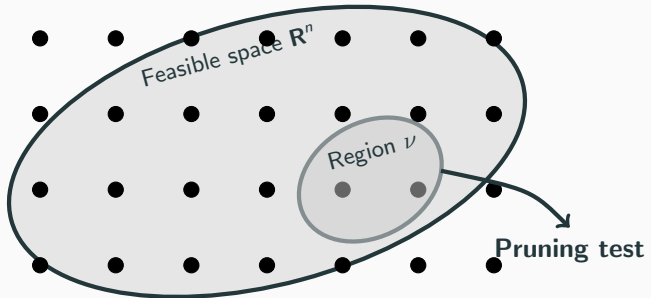
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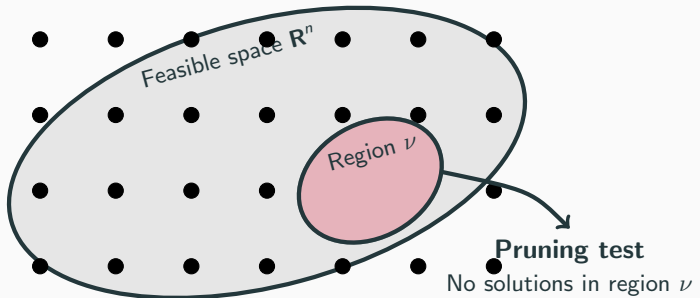
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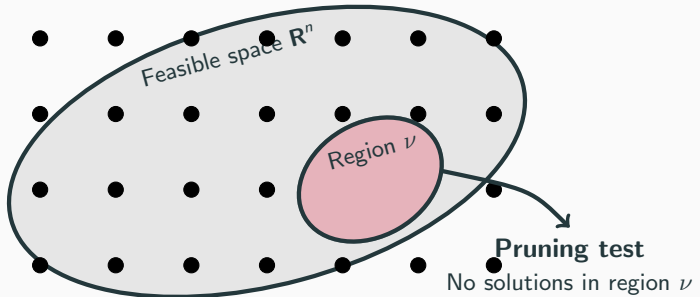
# BnB – Algorithmic principle

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.



**Branching step** – Region design and exploration

**Bounding step** – Pruning test evaluation

### Problem

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



# BnB – Branching step

## Problem

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

## Observation

Solutions are expected  
to be sparse

# BnB – Branching step

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## Method

Drive the sparsity of the  
optimization variable

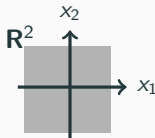
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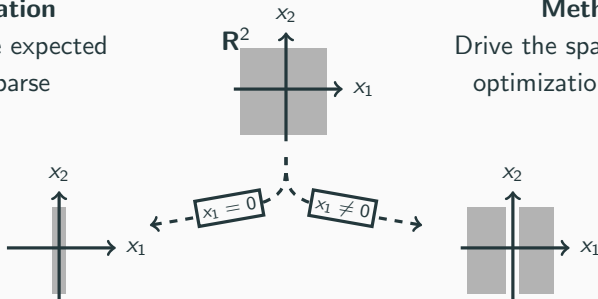
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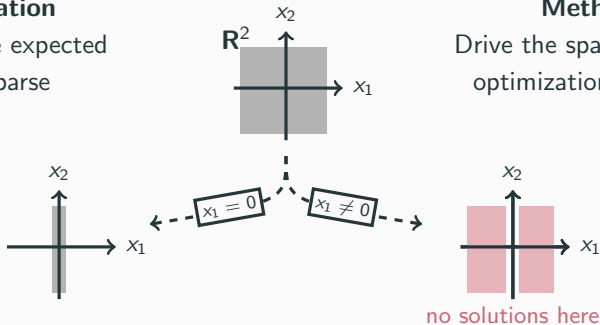
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# BnB – Branching step

## Problem

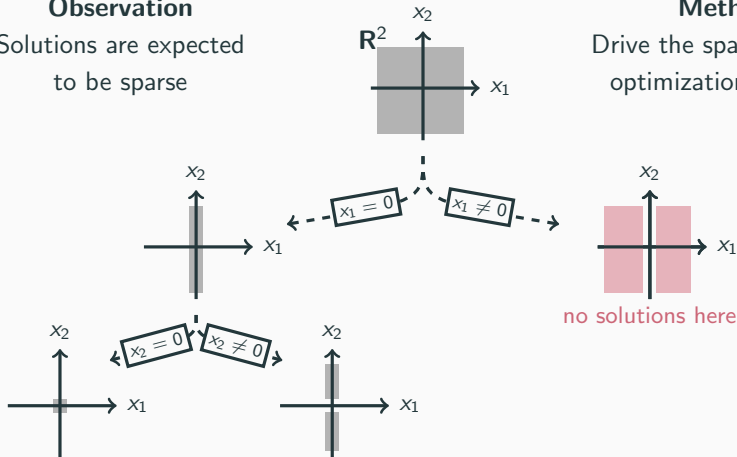
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# BnB – Branching step

## Problem

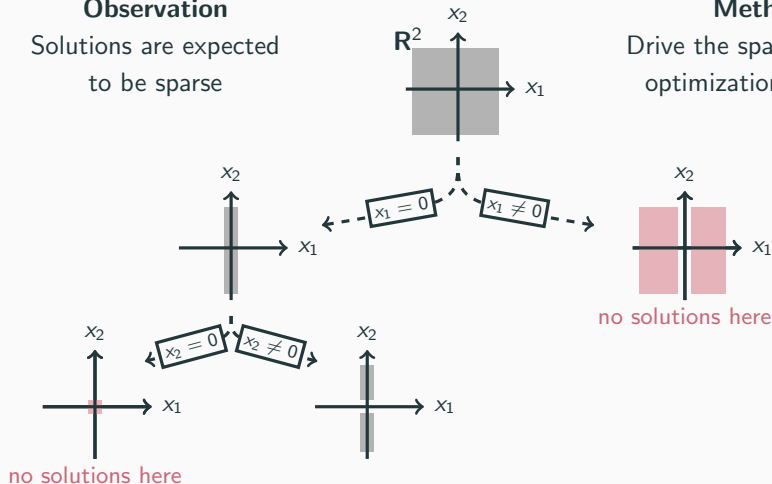
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## Problem

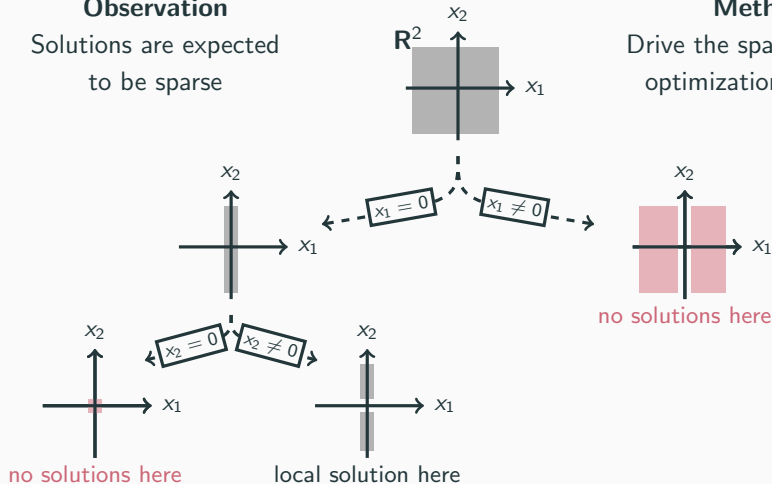
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## Method

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# BnB – Branching step

## Problem

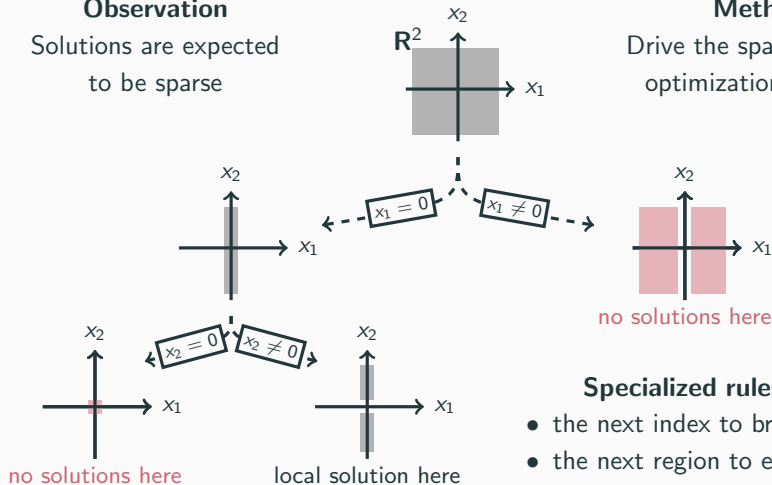
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## Observation

Solutions are expected to be sparse

## Method

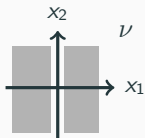
Drive the sparsity of the optimization variable



## Specialized rules for

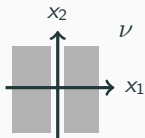
- the next index to branch on
- the next region to explore

## BnB – Bounding step



Does region  $\nu$  contains optimal solutions ?

## BnB – Bounding step

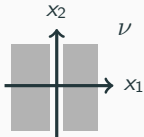


Does region  $\nu$  contains optimal solutions ?

### Problem

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

## BnB – Bounding step



Does region  $\nu$  contains optimal solutions ?

### Problem

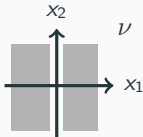
$$p^* = \min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

restrict to  $\nu$

### Restriction to region $\nu$

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

# BnB – Bounding step



Does region  $\nu$  contains optimal solutions ?

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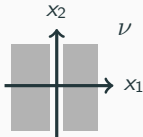
$$p^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

compare

## Pruning test

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

# BnB – Bounding step



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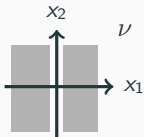
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## Pruning test

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

→ prune  $\nu$

# BnB – Bounding step



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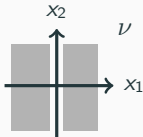
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## Pruning test

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

→ prune  $\nu$

# BnB – Bounding step



Does region  $\nu$  contains optimal solutions ?

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

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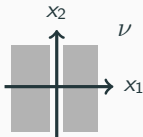
→ prune  $\nu$

## Easy task

Compute an upper bound on  $p^*$



# BnB – Bounding step



Does region  $\nu$  contains optimal solutions ?

## Problem

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

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## Restriction to region $\nu$

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

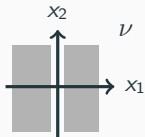
→ prune  $\nu$

## Easy task

Compute an upper bound on  $p^*$

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

# BnB – Bounding step



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## Restriction to region $\nu$

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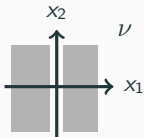
Compute an upper bound on  $p^*$

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

## Main challenge

Compute a lower bound on  $p^\nu$

# BnB – Bounding step



Does region  $\nu$  contains optimal solutions ?

## Problem

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

restrict to  $\nu$

## Restriction to region $\nu$

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

compare

## Pruning test

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

→ prune  $\nu$

## Easy task

Compute an upper bound on  $p^*$

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

## Main challenge

Compute a lower bound on  $p^\nu$

Construct and  
solve a **relaxation**

**Restriction to region  $\nu$**

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

seek **tight/tractable** lower bound on  $p^\nu$

# BnB – Building relaxations

Restriction to region  $\nu$

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

reformulation

Restriction to region  $\nu$

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

seek **tight/tractable** lower bound on  $p^\nu$

with  $g^\nu$  proper and closed

# BnB – Building relaxations

Restriction to region  $\nu$

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

reformulation

Restriction to region  $\nu$

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

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

Relaxation for region  $\nu$

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

seek **tight/tractable** lower bound on  $p^\nu$

with  $g^\nu$  proper and closed

set  $g_{\text{lb}}^\nu$  set as the **convex envelope** of  $g^\nu$

[XXX]

### Solve time


region processing time  $\times$  number of regions processed



# BnB – The secrete sauce

**Solve time**

region processing time × number of regions processed




**Relaxation for region  $\nu$**

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

# BnB – The secrete sauce

## Solve time

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


### Relaxation for region $\nu$

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

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

# BnB – The secrete sauce

Solve time

region processing time × number of regions processed



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This is a **convex** sparse  
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→ first-order methods

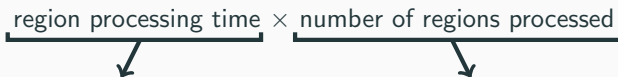
proximal gradient, coordinate descent, ...

→ acceleration strategies

working set, screening tests, ...

# BnB – The secrete sauce

Solve time

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


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Simultaneous pruning

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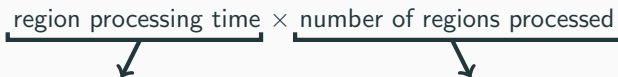
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processing region ...

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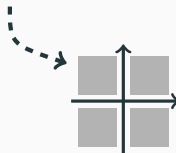
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### Simultaneous pruning



processing region ...



perform **degraded** but  
**low-cost** pruning test

# BnB – The secrete sauce

## Solve time

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

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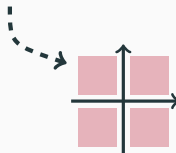
→ acceleration strategies

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### Simultaneous pruning



processing region ...

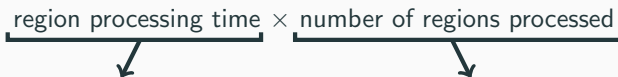


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# BnB – The secrete sauce

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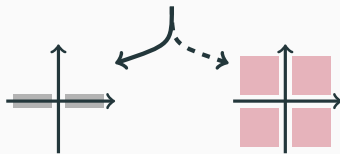
→ acceleration strategies

working set, screening tests, ...

### Simultaneous pruning



processing region ...



continue  
processing

perform **degraded** but  
**low-cost** pruning test

# BnB – The secrete sauce

## Solve time

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

### Relaxation for region $\nu$

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

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This is a **convex** sparse optimization problem

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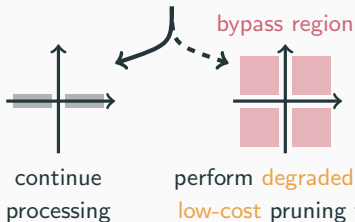
→ acceleration strategies

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### Simultaneous pruning



processing region ...



## Problem

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

## Pipeline

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

# BnB – Let's sum up

## Problem

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

## Pipeline

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## Pros

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

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## Pros

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

## Cons

- ✗ Less standard pipeline

# Conclusion

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# A community with a bunch of people

Non-exhaustive list

# A community with a bunch of people

Non-exhaustive list



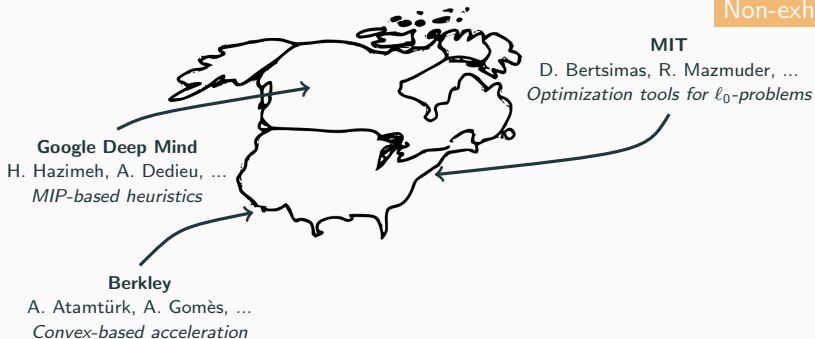
MIT

D. Bertsimas, R. Mazmuder, ...  
*Optimization tools for  $\ell_0$ -problems*



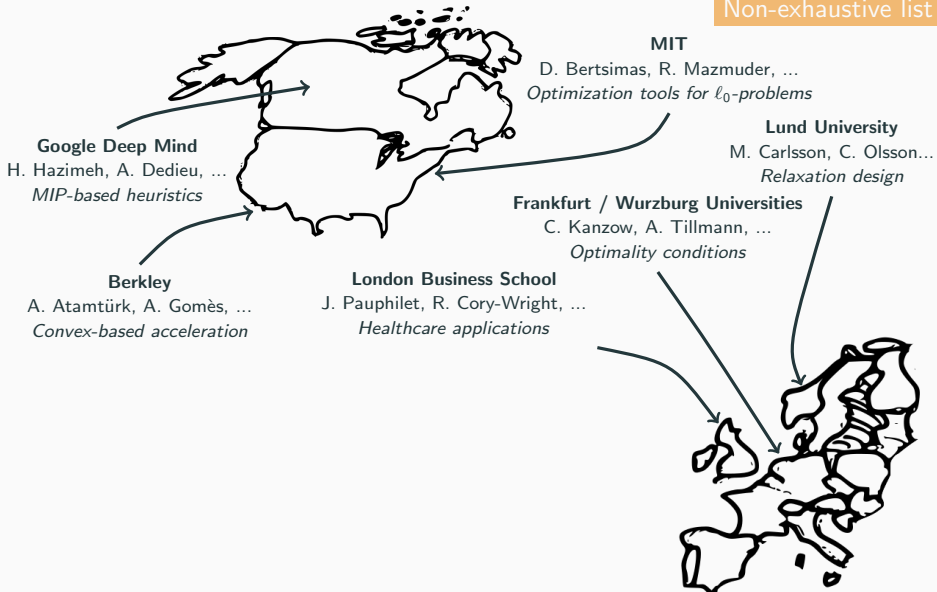
# A community with a bunch of people

Non-exhaustive list



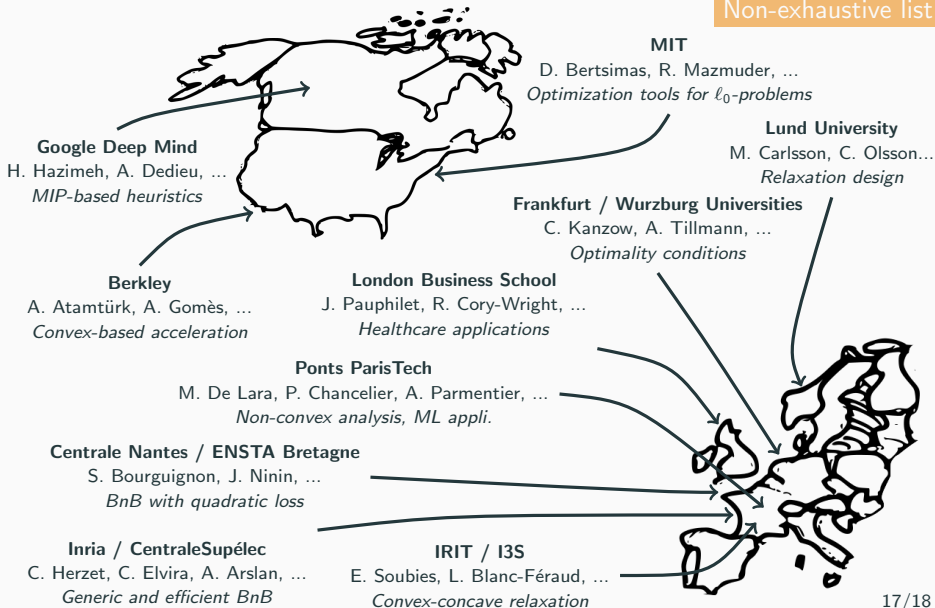
# A community with a bunch of people

Non-exhaustive list



# A community with a bunch of people

Non-exhaustive list



# Take-home messages

- Although NP-hard,  $\ell_0$ -problems are of practical interest
- There exists methods to tackle them exactly
  - MIP-based formulation and off-the-shelf solvers
  - Specialized BnB algorithms
  - Structure-exploitation is key
- It's an active research area
  - Theoretical and methodological developments missing
  - Need to reach the application world

Question time !



# Compressed sensing

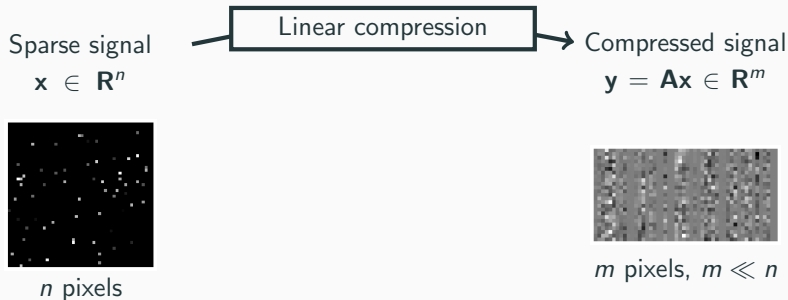
Sparse signal

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

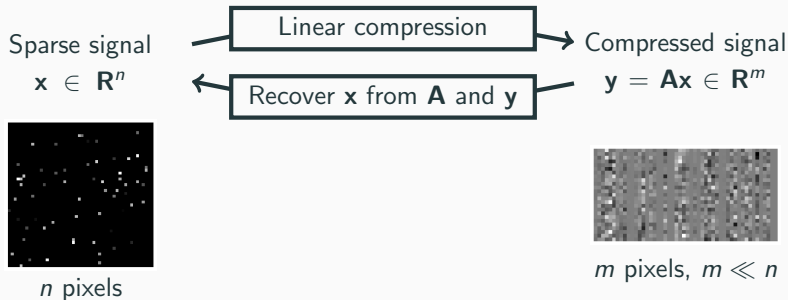


$n$  pixels

# Compressed sensing

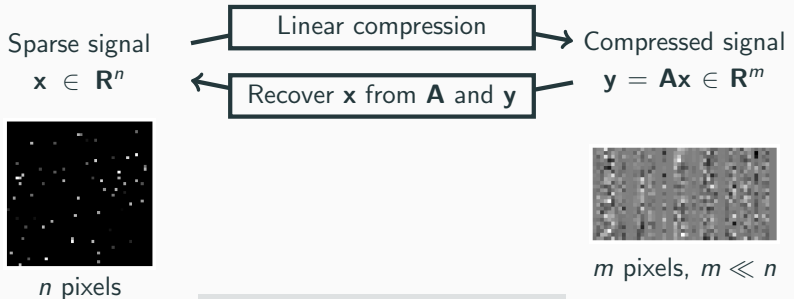


# Compressed sensing





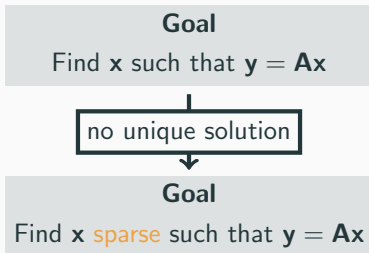
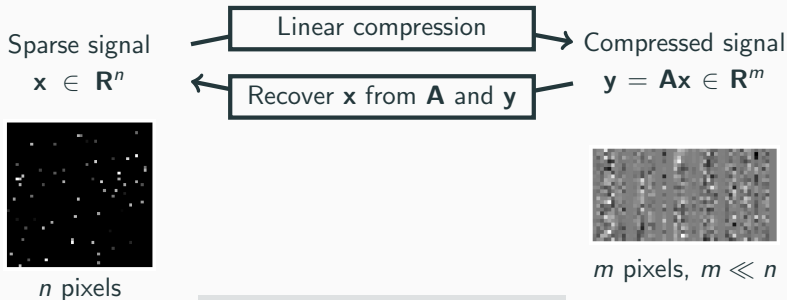
# Compressed sensing



## Goal

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

# Compressed sensing



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

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

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**Model accuracy**

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

**Model explainability**

Use few features

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Model explainability

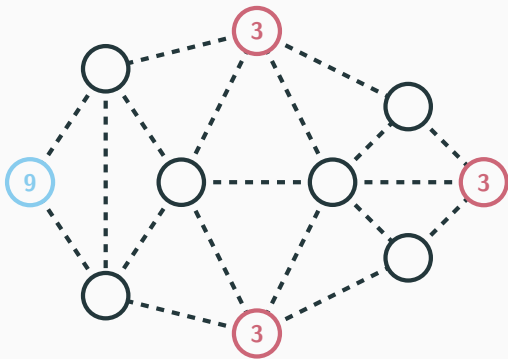
Use few features



Goal

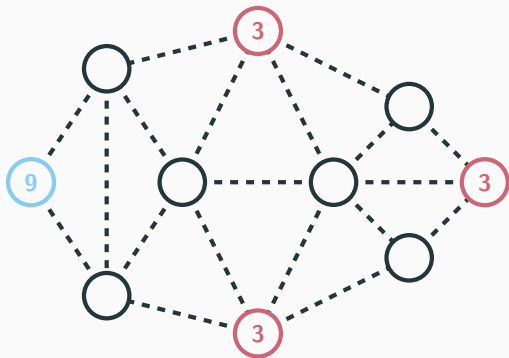
Find  $\mathbf{x}$  **sparse** such that  $\mathcal{L}_\phi(\mathbf{Ax}, \mathbf{y})$  is small

# Network design



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

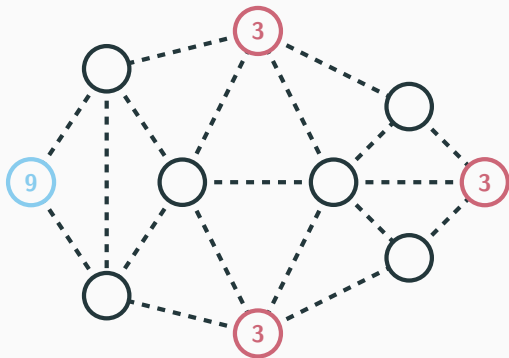
# Network design



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# Network design

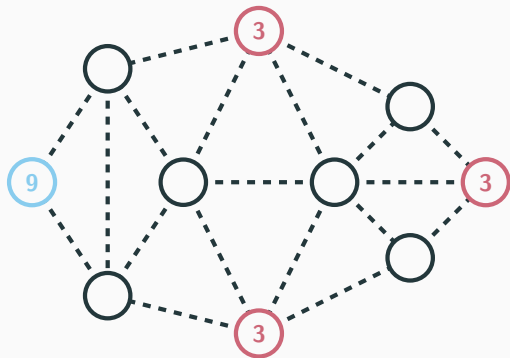


Which edges to build to transport products from **source** to **sink** nodes ?



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

# Network design



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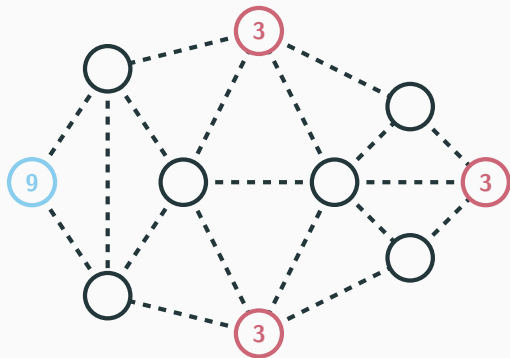


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## Question

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

# 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  $c$

## Question

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



Find  $\mathbf{x} \in \mathbf{R}^{\text{card}(I)}$  **sparse**  
such that  $Q(\mathbf{x}) = 0$

# 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	<b>-6.64</b>
#2	7.29	6.39	11.32	9.42	...	6.99	<b>-5.43</b>
...	...	...	...	...	...	...	...
#71	6.85	8.27	7.98	8.04	...	6.65	<b>-7.58</b>

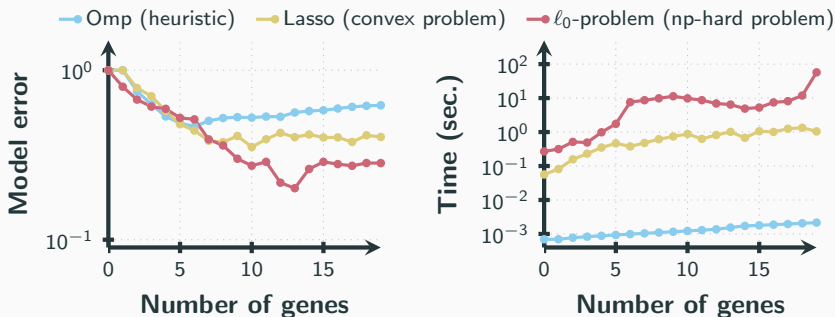
4,088 genes

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## Sparse regression

Find  $\mathbf{x}$  sparse such  
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## Optimization problem

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

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

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## MIP formulation

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



```
$ pip install cvxpy
```

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# MIP – Hands-on with cvxpy

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

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```
$ pip install e10ps
```

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```
from e10ps.datafits import LeastSquares
from e10ps.penalties import Bigm
from e10ps.solvers import BnbSolver
```

```
# Generate sparse regression data
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```

```
$ pip install el0ps
```

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from el0ps.datafits import LeastSquares
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```

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

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

```
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## Sparse regression

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# Instantiate the loss and penalty
f = LeastSquares(A, y)
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```

```
# Solve the problem with el0ps' solver
solver = BnbSolver()
solver.solve(f, h, lmbd=0.01)
```