

Optimization methods for ℓ_0 -problems

Théo Guyard

JOPT, HEC Montréal, Canada – May 12th, 2025

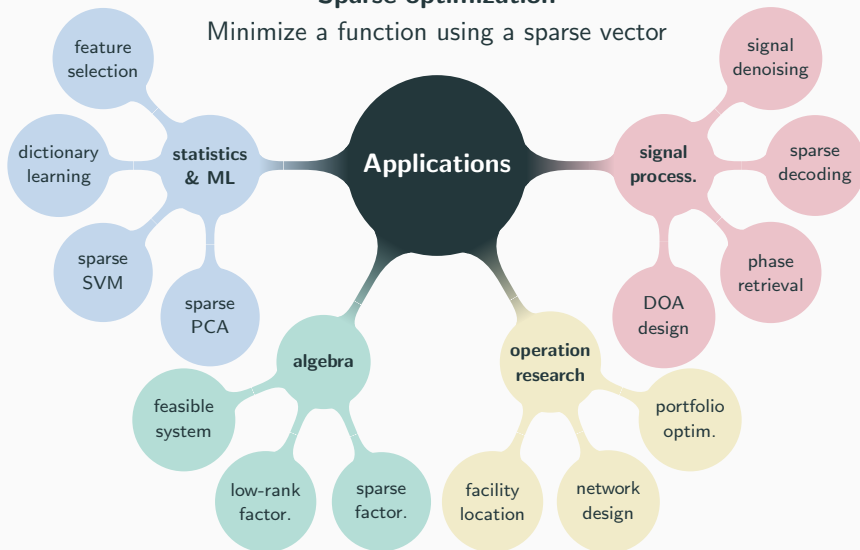
Sparse optimization

Minimize a function using a sparse vector

Sparse optimization

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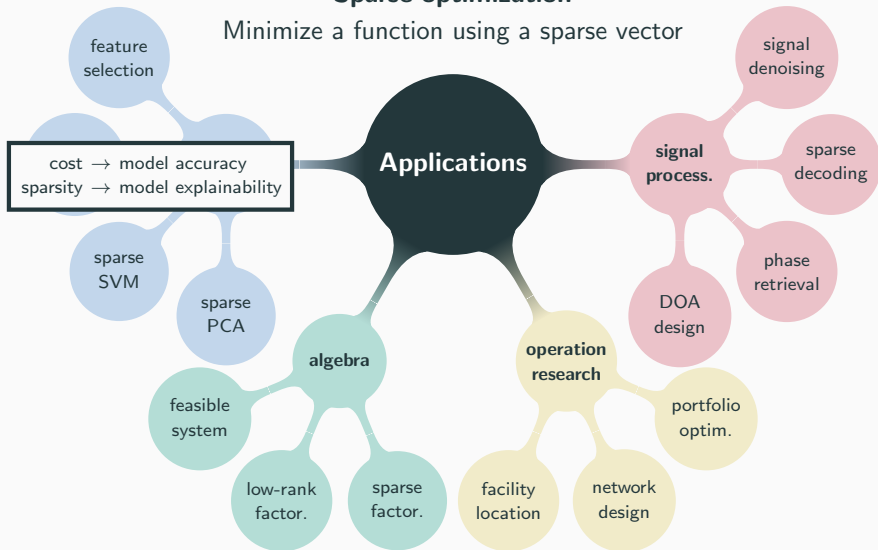
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Sparse optimization

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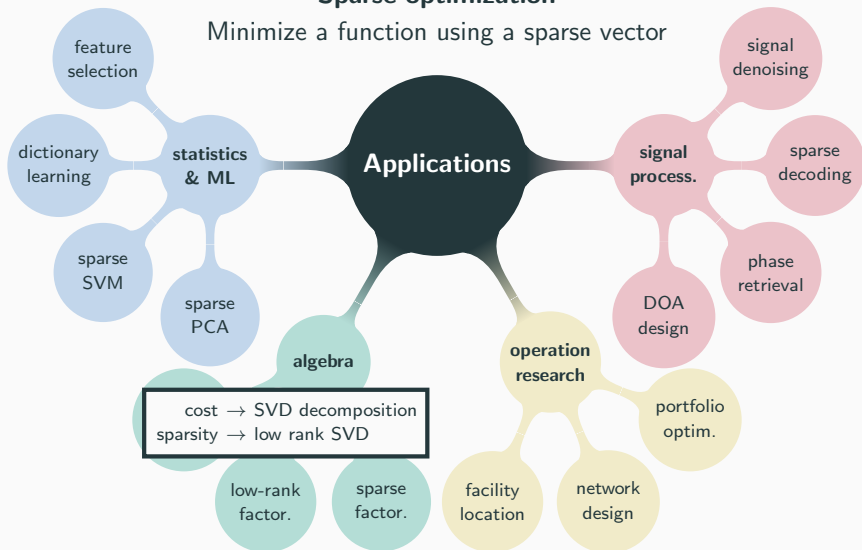
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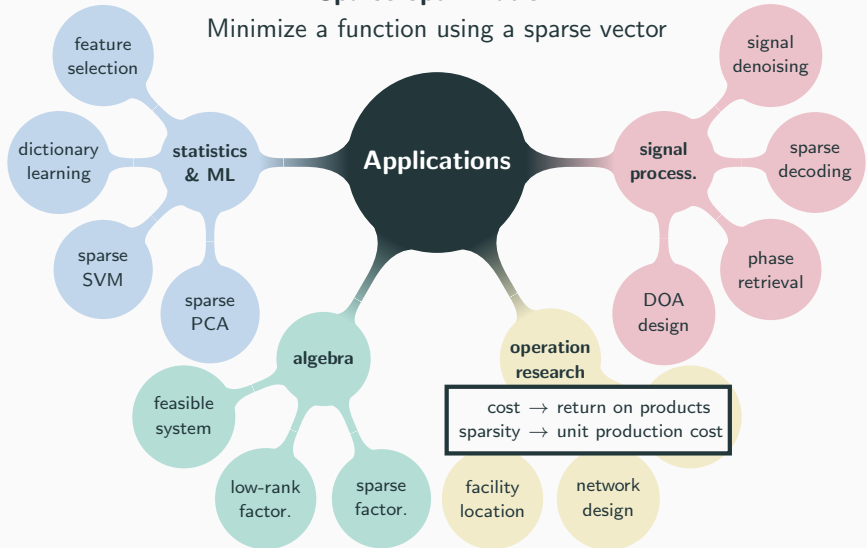
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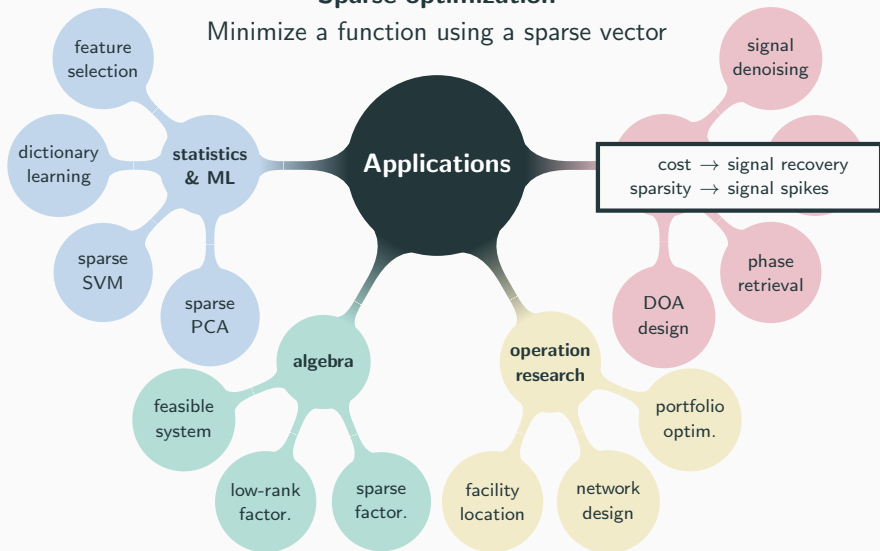
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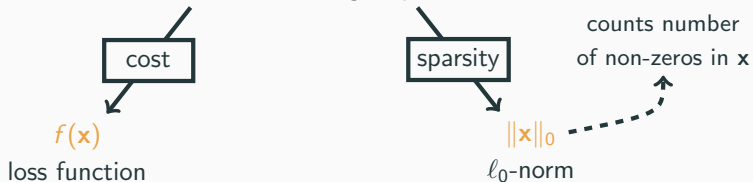
$f(\mathbf{x})$

loss function

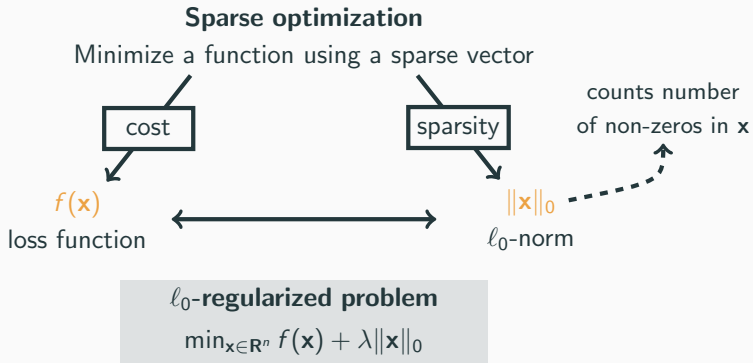
ℓ_0 -regularized problems

Sparse optimization

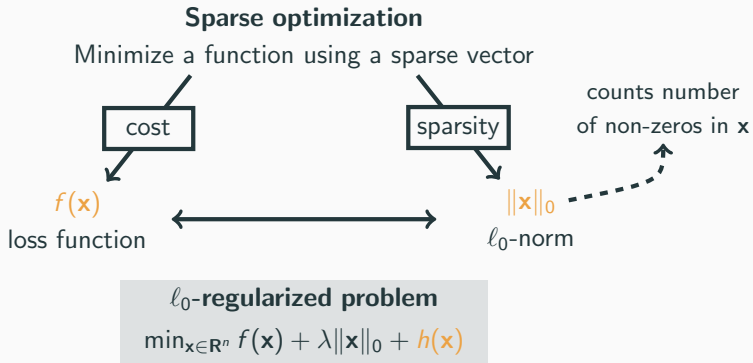
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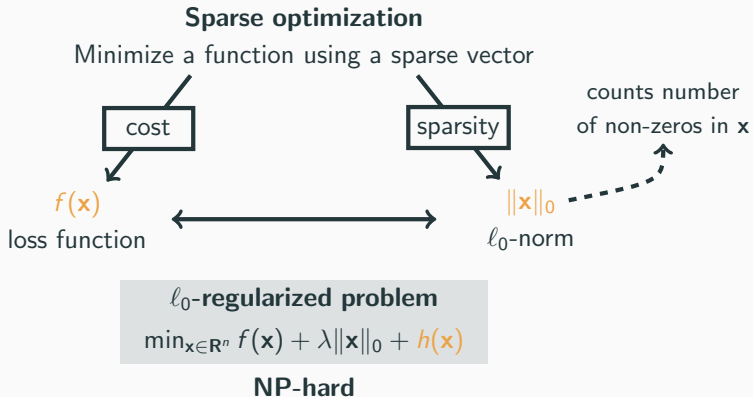
ℓ_0 -regularized problems



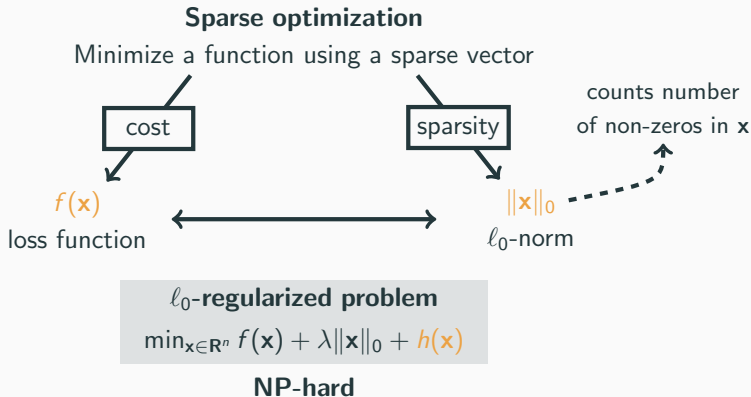
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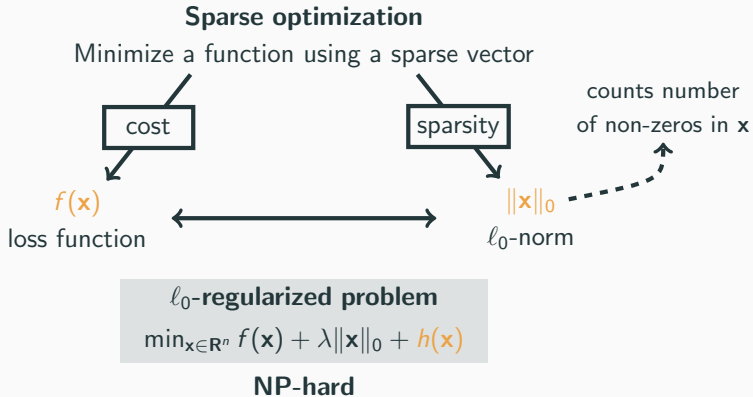
ℓ_0 -regularized problems



Off-the-shelf MIP solvers

- ✗ Poor numerical performances
- ✗ Need standardized expressions

ℓ_0 -regularized problems



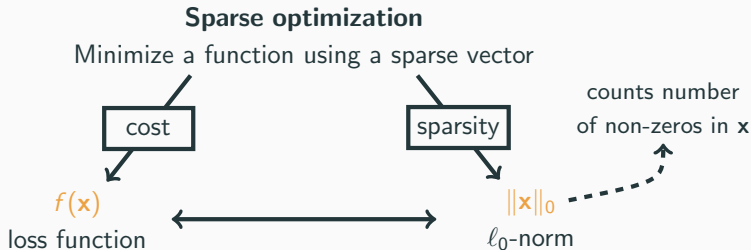
Off-the-shelf MIP solvers

- ✗ Poor numerical performances
- ✗ Need standardized expressions

Specialized Branch-and-Bound

- ✓ Better numerical performances
- ✓ Greater flexibility

ℓ_0 -regularized problems



ℓ_0 -regularized problem

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

NP-hard

Off-the-shelf MIP solvers

- ✗ Poor numerical performances
- ✗ Need standardized expressions

Topic of this talk

Specialized Branch-and-Bound

- ✓ Better numerical performances
- ✓ Greater flexibility

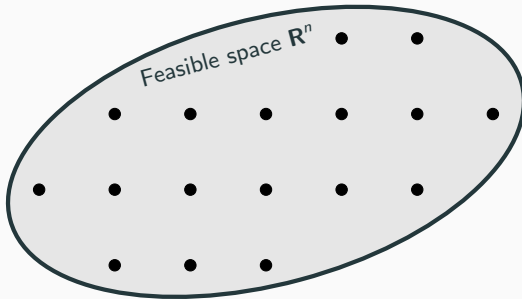
Branch-and-Bound Algorithms

BnB – Algorithmic principle

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

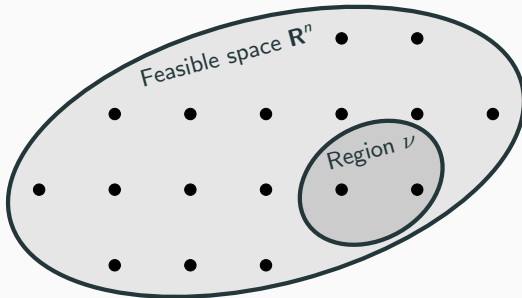
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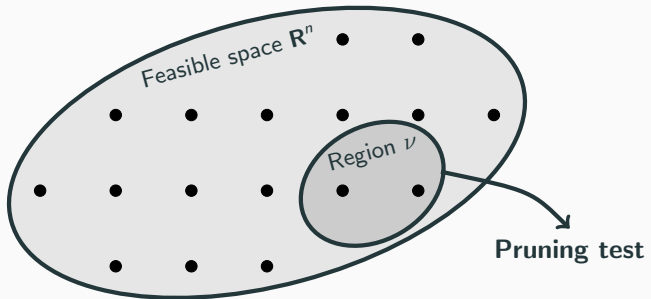
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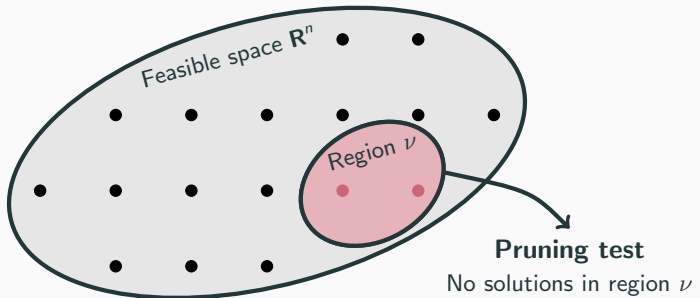
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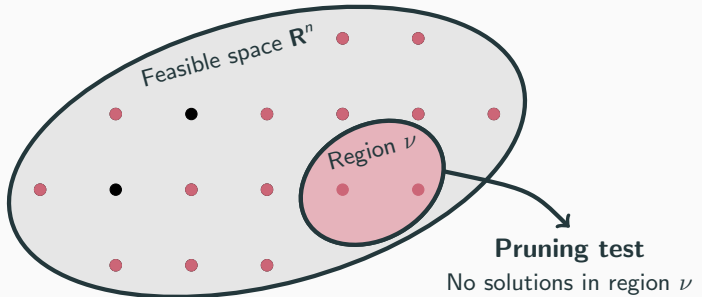
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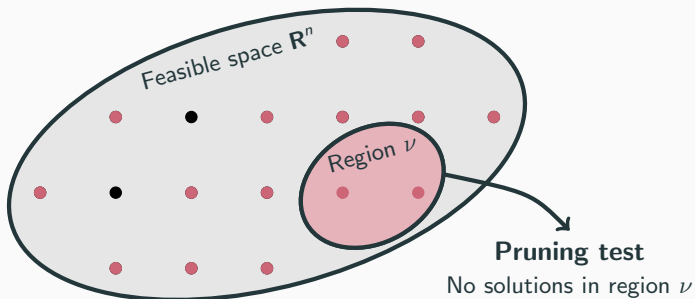
BnB – Algorithmic principle

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

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

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

Problem

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

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Method

Drive the sparsity of the
optimization variable

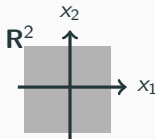
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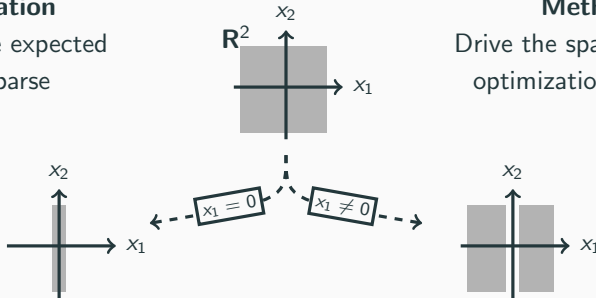
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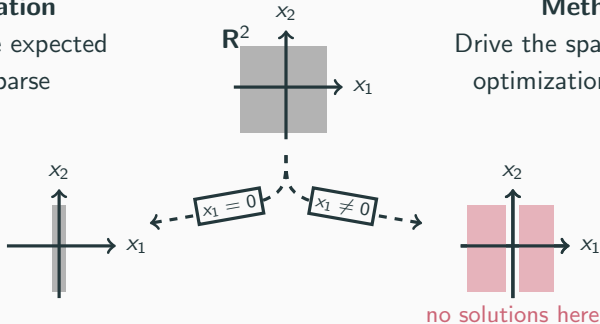
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Problem

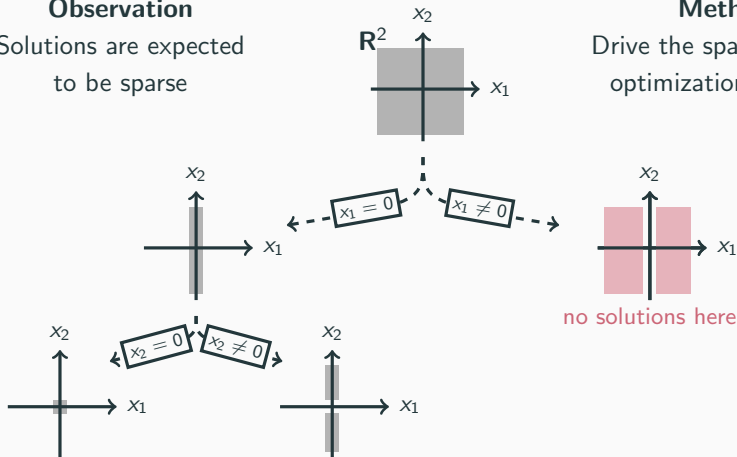
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BnB – Branching step

Problem

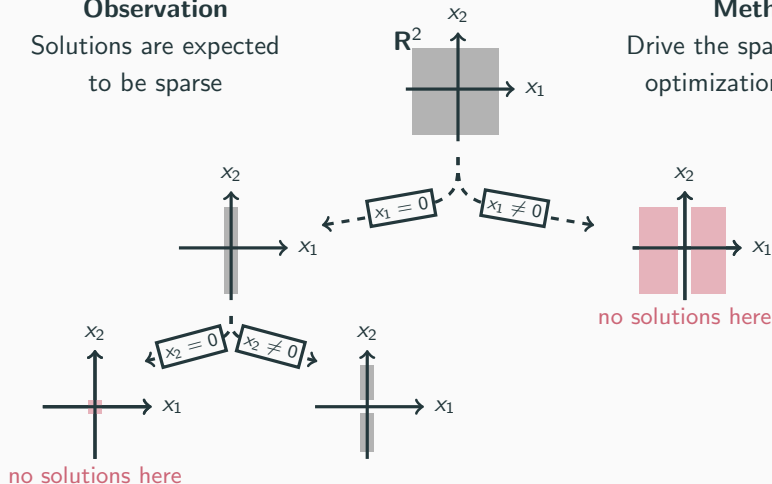
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BnB – Branching step

Problem

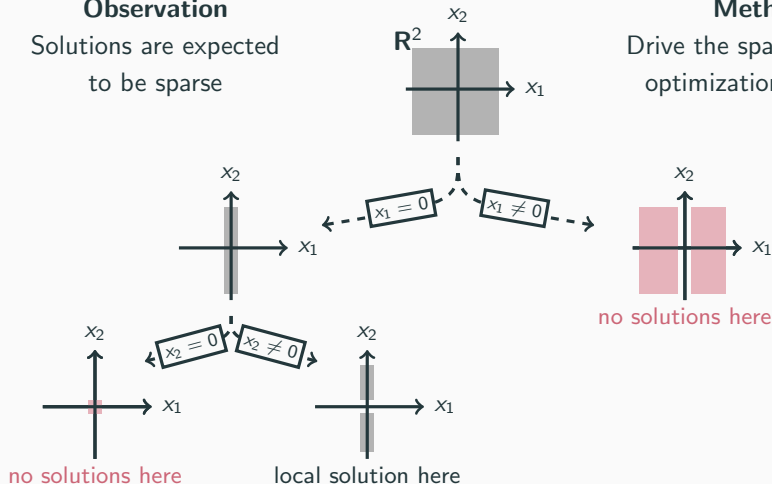
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Drive the sparsity of the optimization variable



BnB – Branching step

Problem

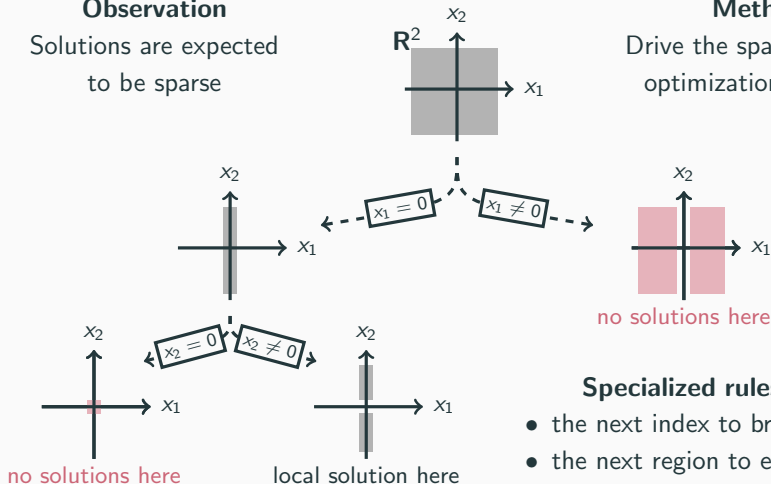
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Observation

Solutions are expected to be sparse

Method

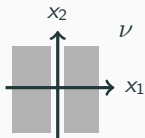
Drive the sparsity of the optimization variable



Specialized rules for

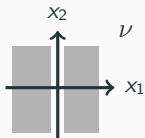
- the next index to branch on
- the next region to explore

BnB – Bounding step



Does region ν contains optimal solutions ?

BnB – Bounding step

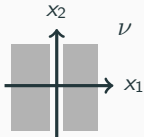


Does region ν contains optimal solutions ?

Problem

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

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

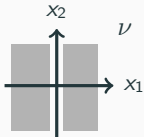
$$p^* = \min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

restrict to ν

Restriction to region ν

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

BnB – Bounding step



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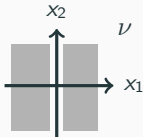
$$p^\nu = \min_{\mathbf{x} \in \nu} f(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 + h(\mathbf{x})$$

compare

Pruning test

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

BnB – Bounding step



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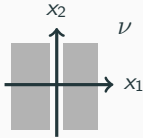
compare

Pruning test

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

→ prune ν

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

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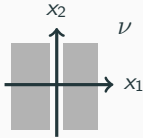
compare

Pruning test

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

→ prune ν

BnB – Bounding step



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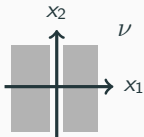
$$p_{\text{lb}}^\nu > p_{\text{ub}}^*$$

→ prune ν

Easy task

Compute an upper bound on p^*

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

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

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

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

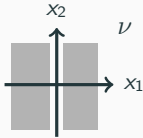
→ prune ν

Easy task

Compute an upper bound on p^*

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

BnB – Bounding step



Does region ν contains optimal solutions ?

Problem

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restrict to ν

Restriction to region ν

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compare

Pruning test

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

→ prune ν

Easy task

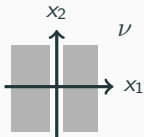
Compute an upper bound on p^*

Construct and evaluate
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Main challenge

Compute a lower bound on p^ν

BnB – Bounding step



Does region ν contains optimal solutions ?

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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

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

→ prune ν

Easy task

Compute an upper bound on p^*

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

Main challenge

Compute a lower bound on p^ν

Construct and
solve a **relaxation**

BnB – Building relaxations

Restriction to region ν

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

seek **tight/tractable** lower bound on p^ν

BnB – Building relaxations

Restriction to region ν

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

reformulation

Restriction to region ν

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

seek **tight/tractable** lower bound on p^ν

with g^ν proper and closed

BnB – Building relaxations

Restriction to region ν

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reformulation

Restriction to region ν

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

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

Relaxation for region ν

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

seek **tight/tractable** lower bound on p^ν

with g^ν proper and closed

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

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

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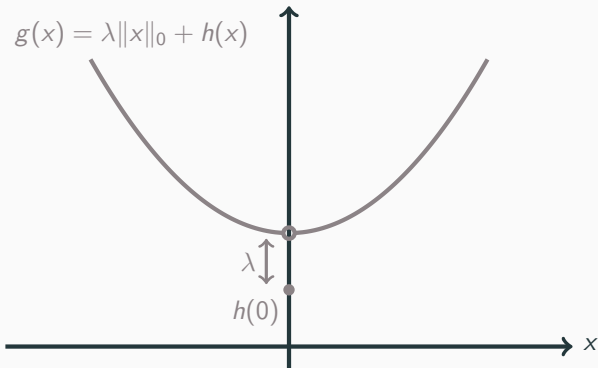
Convex envelope of $g(x) = \lambda \|x\|_0 + h(x)$ with $x \in \mathbb{R}$

BnB – Geometrical intuition

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



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

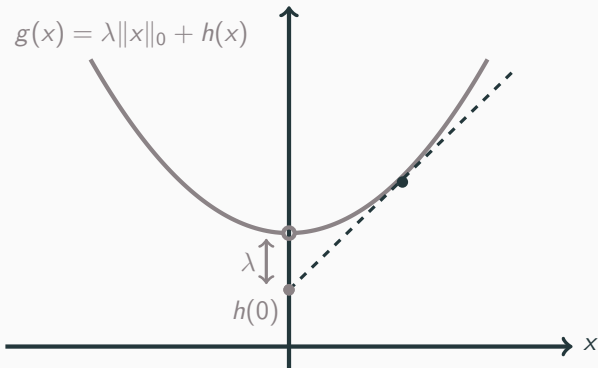


BnB – Geometrical intuition

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

h separable

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

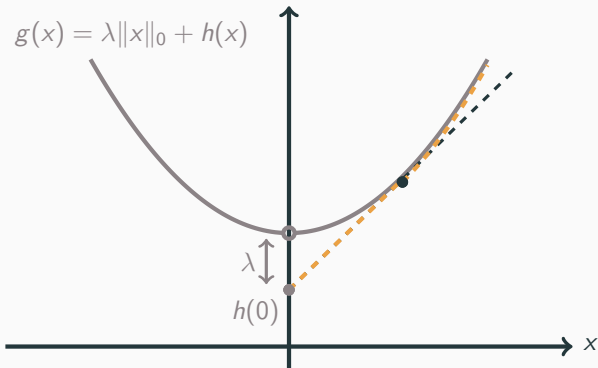


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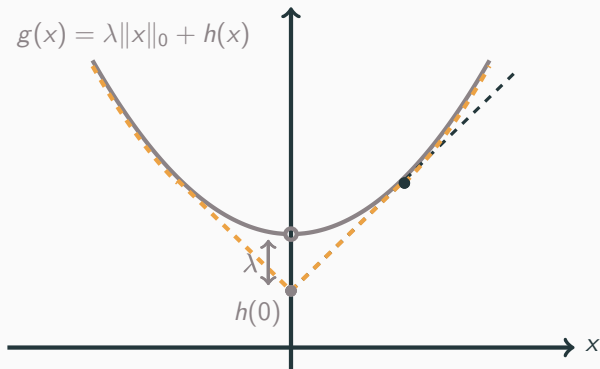


BnB – Geometrical intuition

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




Overall solve time

pruning test time \times number of regions processed

BnB – The secrete sauce

Overall solve time

$$\text{pruning test time} \times \text{number of regions processed}$$


Relaxation for region ν

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

Overall solve time

$$\frac{\text{pruning test time} \times \text{number of regions processed}}{\downarrow}$$


Relaxation for region ν

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

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

BnB – The secrete sauce

Overall solve time

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This is a **convex** sparse
optimization problem

BnB – The secrete sauce

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→ first-order methods

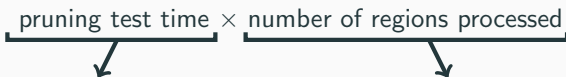
proximal gradient, coordinate descent, ...

→ acceleration strategies

working set, screening tests, ...

BnB – The secrete sauce

Overall solve time

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Relaxation for region ν

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

Simultaneous pruning

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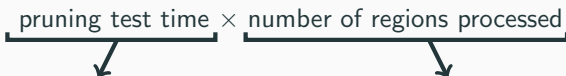
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BnB – The secrete sauce

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→ acceleration strategies

working set, screening tests, ...

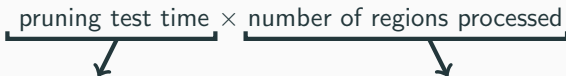
Simultaneous pruning



processing region ...

BnB – The secrete sauce

Overall solve time

$$\underbrace{\text{pruning test time}} \times \underbrace{\text{number of regions processed}}$$


Relaxation for region ν

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

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



This is a **convex** sparse
optimization problem

→ first-order methods

proximal gradient, coordinate descent, ...

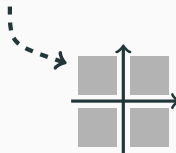
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perform **degraded** but
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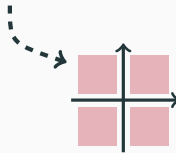
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Simultaneous pruning



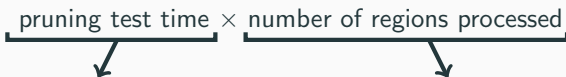
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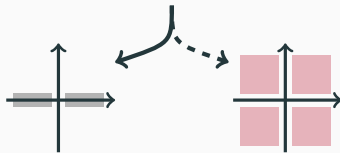
→ acceleration strategies

working set, screening tests, ...

Simultaneous pruning



processing region ...




continue
processing

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

BnB – The secret sauce

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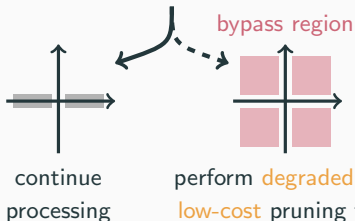
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processing region ...



Numerical Illustration

Numerics – Feature Selection Problem

Problem

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

MIP solvers:  cplex  mosek

BnB solver:  e10ps

Numerics – Feature Selection Problem

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

MIP solvers:  cplex  mosek

BnB solver:  e10ps

Instance 1

- f : LeastSquares($\mathbf{y}, \mathbf{A}\mathbf{x}$)
- h : ℓ_2 -norm + bound constraint on \mathbf{x}
- riboflavin: $\mathbf{y} \in \mathbb{R}^{71}$ and $\mathbf{A} \in \mathbb{R}^{71 \times 4088}$

Numerics – Feature Selection Problem

Problem

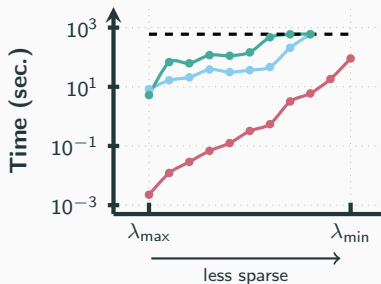
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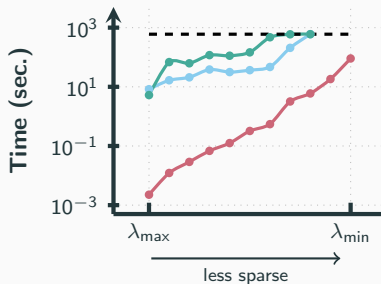
BnB solver: e10ps

Instance 1

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- riboflavin: $\mathbf{y} \in \mathbb{R}^{71}$ and $\mathbf{A} \in \mathbb{R}^{71 \times 4088}$

Instance 2

- f : Logistic(\mathbf{y}, \mathbf{Ax})
- h : ℓ_1 -norm + bound constraint on \mathbf{x}
- leukemia: $\mathbf{y} \in \mathbb{B}^{38}$ and $\mathbf{A} \in \mathbb{R}^{38 \times 7129}$



Numerics – Feature Selection Problem

Problem

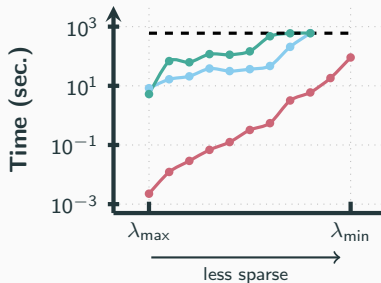
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MIP solvers: cplex mosek

BnB solver: e10ps

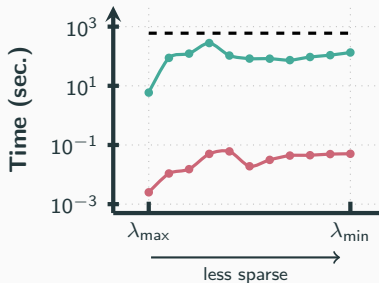
Instance 1

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Instance 2

- f : Logistic($\mathbf{y}, \mathbf{A}\mathbf{x}$)
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- leukemia: $\mathbf{y} \in \mathbb{B}^{38}$ and $\mathbf{A} \in \mathbb{R}^{38 \times 7129}$



Take-home messages

- ℓ_0 -problems are of great practical interest but NP-hard
- Off-the-shelf MIP solvers
 - ✗ Poor numerical performances
 - ✗ Need standardized expressions
- Specialized BnB solvers
 - ✓ Better numerical performances
 - ✓ Greater flexibility
- Structure-exploitation is key
 - Sparsity-driven branching strategy
 - Convexification-based bounding strategy
 - Efficient convex solver for lower bounds
 - Dedicated simultaneous pruning strategy

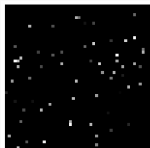
Question time !



Compressed sensing

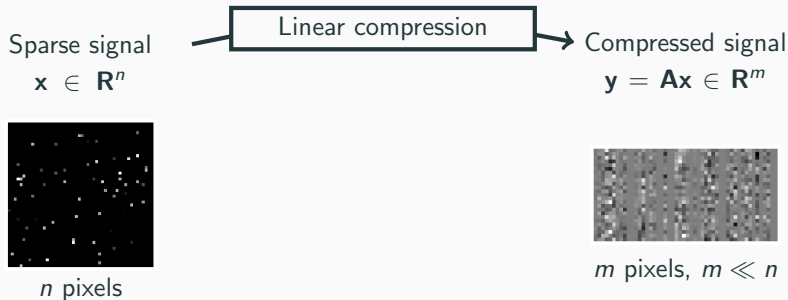
Sparse signal

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

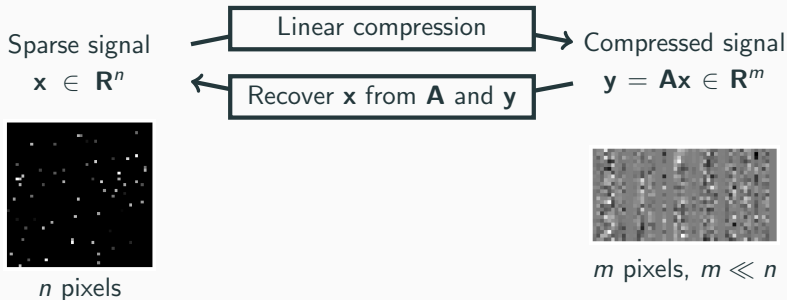


n pixels

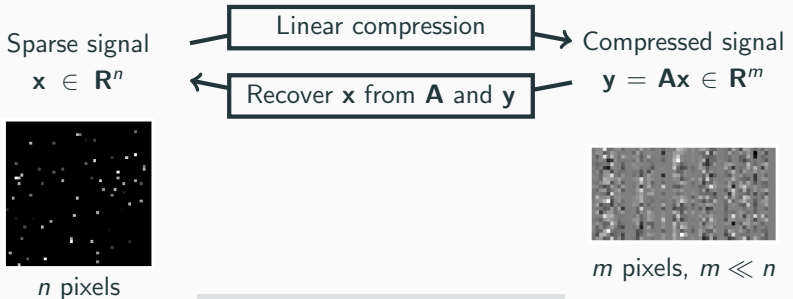
Compressed sensing



Compressed sensing



Compressed sensing



Goal

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

Compressed sensing

Sparse signal

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



n pixels

Linear compression

Compressed signal

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

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



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

Feature selection

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Sample 1	$a_{1,1}$	$a_{1,2}$...	$a_{1,n}$	y_1
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Model explainability

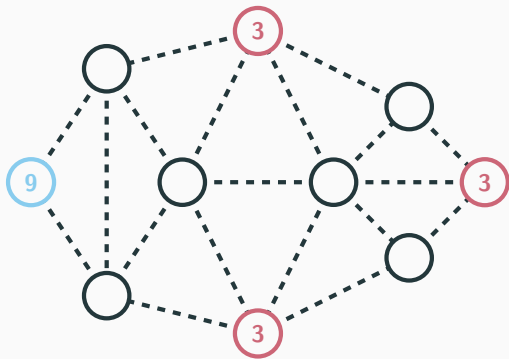
Use few features



Goal

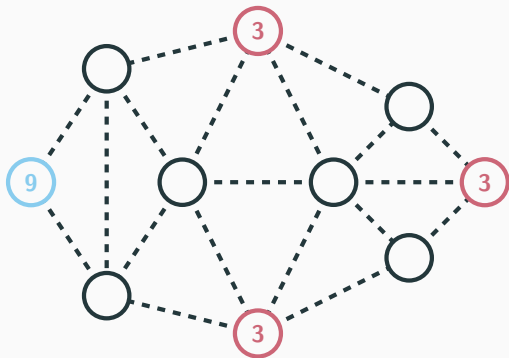
Find \mathbf{x} **sparse** such that $\mathcal{L}_\phi(\mathbf{Ax}, \mathbf{y})$ is small

Network design



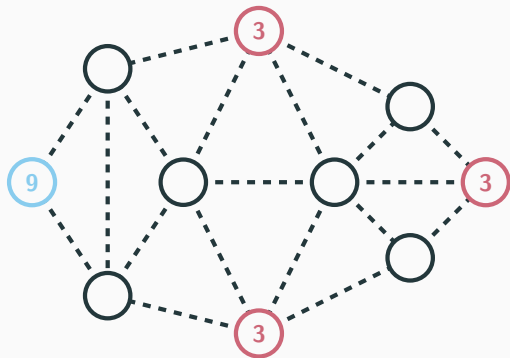
Which edges to build to transport products from **source** to **sink** nodes ?

Network design



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

Network design

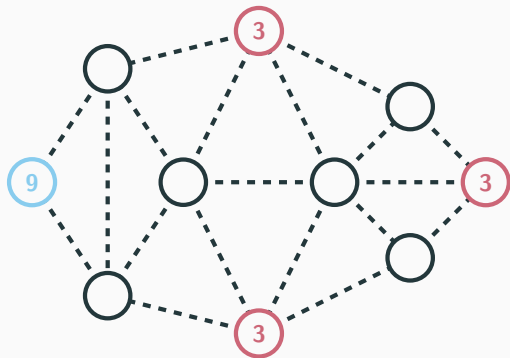


Which edges to build to transport products from **source** to **sink** nodes ?



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 ?

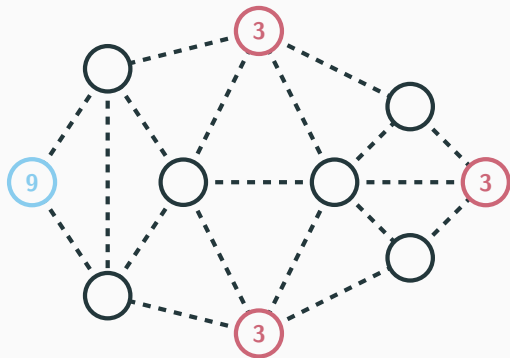


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Question

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

Network design



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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	-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

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