# Optimization methods for $\ell_0$-problems

Théo Guyard

ML MTP – December 9th, 2024

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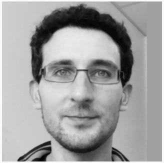


**Cédric Herzet**
Inria/Ensai Rennes

**Clément Elvira**
CentraleSupélec Rennes

**Ayșe-Nur Arslan**
Inria Bordeaux

**Sparse optimization**

Minimize a cost with a sparse solution

# Sparse optimization

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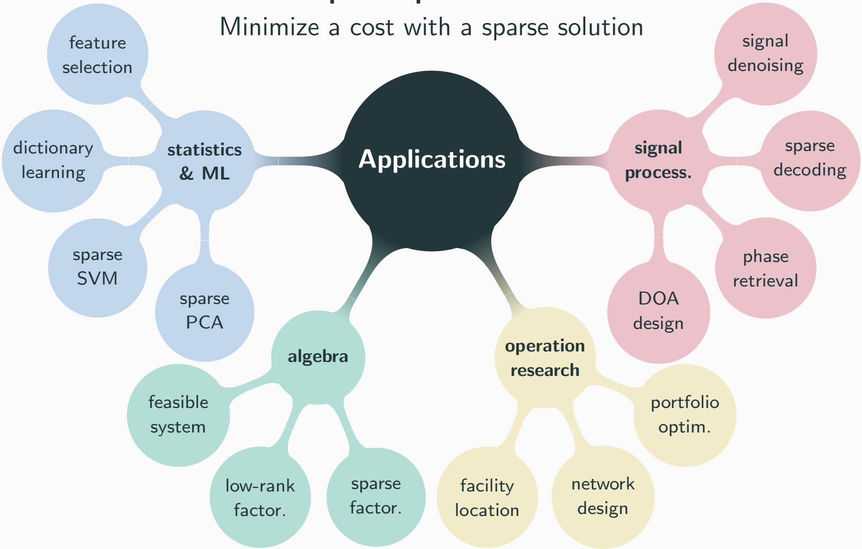


A. Tillmann *et. al* (2024)

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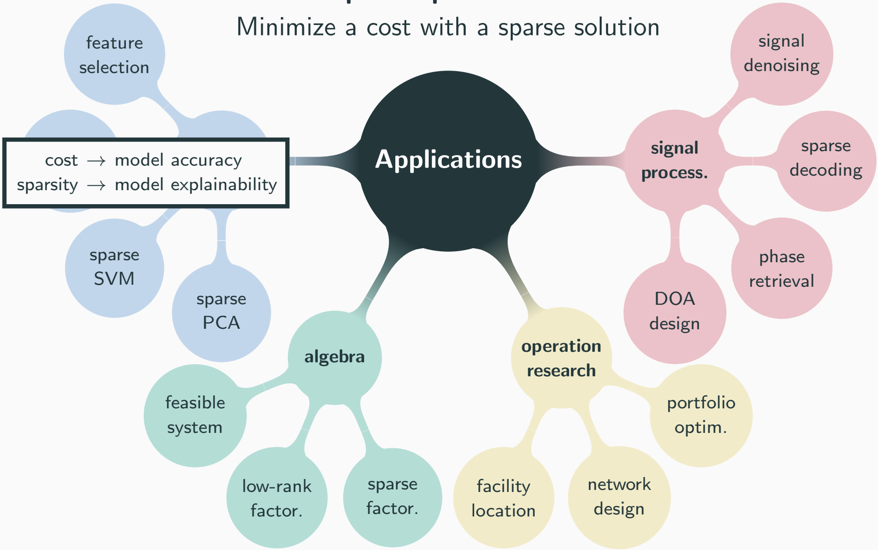


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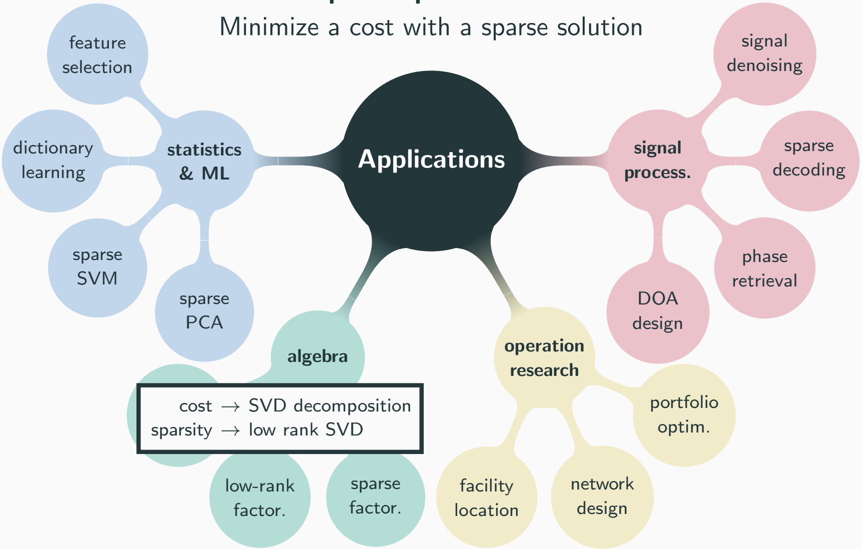


cost $\rightarrow$ SVD decomposition
sparsity $\rightarrow$ low rank SVD

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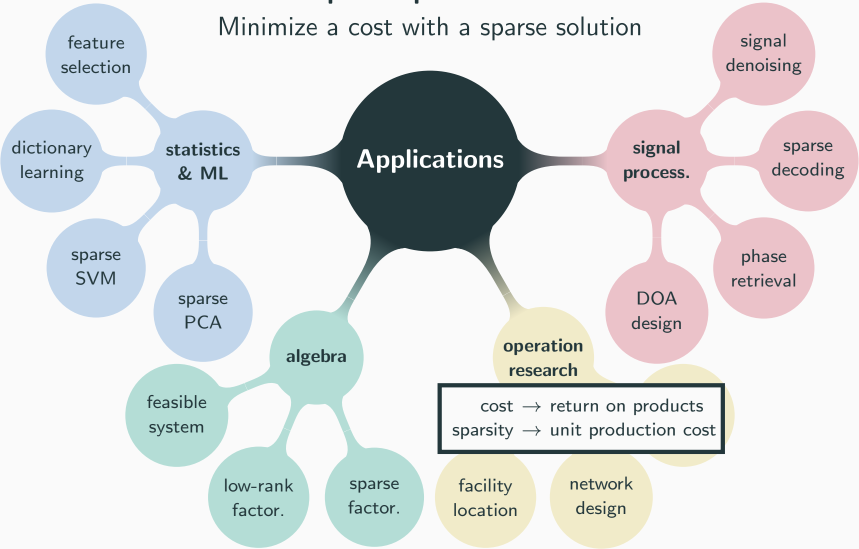


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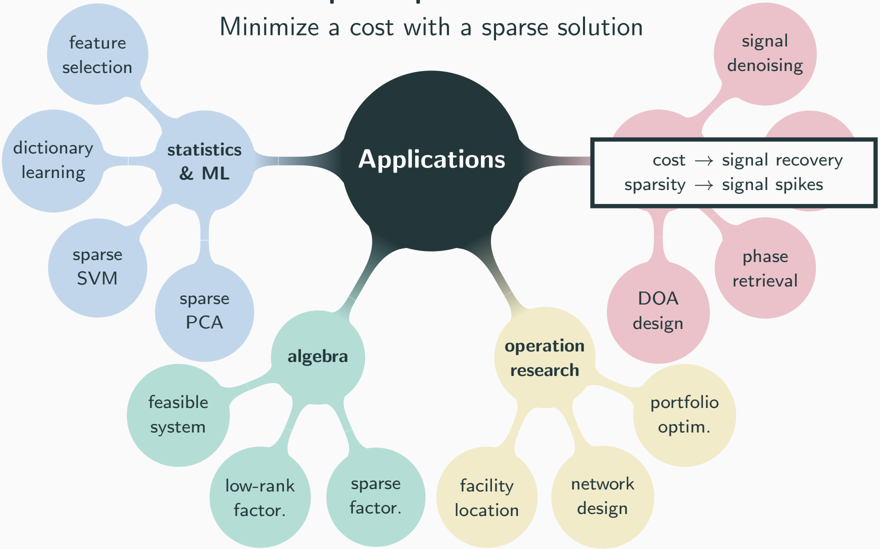


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# Minimized, constrained, or regularized problem ?

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quantify cost

$f(\mathbf{x})$

thing to minimize

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**Constrained version**

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

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**Regularized version**

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

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**Regularized version**

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

# A bit of history

**Problem**

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

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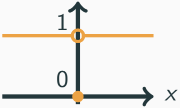
**1d graph**



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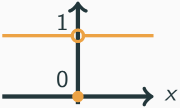


non-convex, non-diff.,
non-continuous, ...

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**NP-hard to solve**

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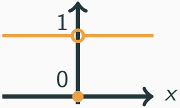


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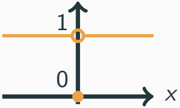


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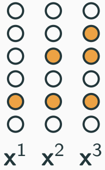
**1995**

Heuristics

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



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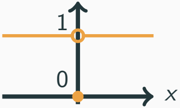


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**2000**

Recovery cond.

RIP, NSP, ...
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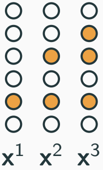


OMP solves
$\ell_0$-problem
under RIP

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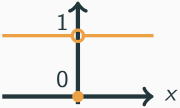


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**1995** — Heuristics
MP, OMP, ...
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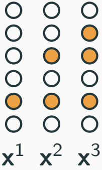
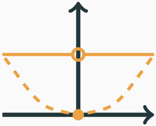
**2005** — Convex approx.
Lasso, Elastic-Net, ...
R. Tibshirani (2005)




OMP solves $\ell_0$-problem under RIP



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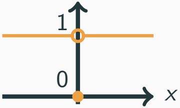


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| **1995** | **2000** | **2005** | **2010** |
|---|---|---|---|
| Heuristics | Recovery cond. | Convex approx. | Concave approx. |
| MP, OMP, ... | RIP, NSP, ... | Lasso, Elastic-Net, ... | SCAD, MCP, ... |
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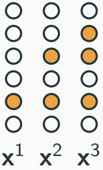


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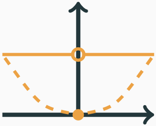

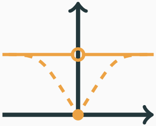

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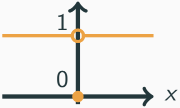


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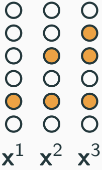
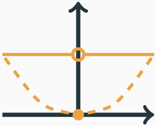
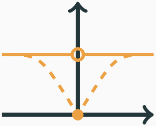
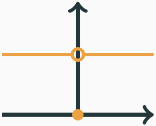
| **1995** | **2000** | **2005** | **2010** | **2015** |
|---|---|---|---|---|
| Heuristics | Recovery cond. | Convex approx. | Concave approx. | Exact methods |
| MP, OMP, ... | RIP, NSP, ... | Lasso, Elastic-Net, ... | SCAD, MCP, ... | MIP, BnB, ... |
| S. Mallat (1993) | E. Candes (2004) | R. Tibshirani (2005) | C. Zhang (2010) | D. Bertsimas (2016) |
|   | OMP solves $\ell_0$-problem under RIP |  |  |  |

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**1) MIP-based methods**

Convenient for practitioners

Poor numerical performances

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Ok, $\ell_0$-problems can be of practical interest !

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Poor numerical performances

**2) Specialized Branch-and-Bound**

More sophisticated mechanism

Better numerical performances

# Topic of this talk

Ok, $\ell_0$-problems can be of practical interest !

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**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**

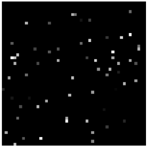
**Question time !**

🤓

# Compressed sensing

Sparse signal

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



$n$ pixels

# Compressed sensing

Sparse signal

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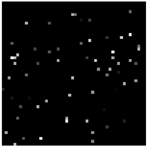

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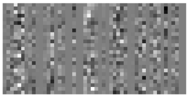
Linear compression

Compressed signal

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



$m$ pixels, $m \ll n$

# Compressed sensing

Sparse signal

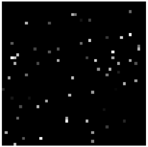
$\mathbf{x} \in \mathbf{R}^n$

Linear compression

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

Compressed signal

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



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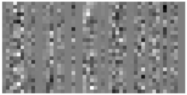

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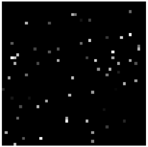

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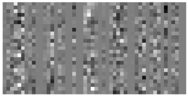

$m$ pixels, $m \ll n$

**Goal**

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

# Compressed sensing

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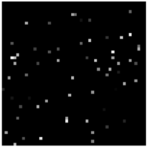

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Recover $\mathbf{x}$ from $\mathbf{A}$ and $\mathbf{y}$

Compressed signal

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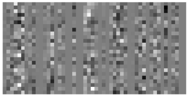

$m$ pixels, $m \ll n$

**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** | $a_{m,1}$ | $a_{m,2}$ | ... | $a_{m,n}$ | $y_m$ |

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

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

**Model explainability**
Use few features

# Feature selection

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| **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** | $a_{m,1}$ | $a_{m,2}$ | $\cdots$ | $a_{m,n}$ | $y_m$ |

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

**Model accuracy**

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

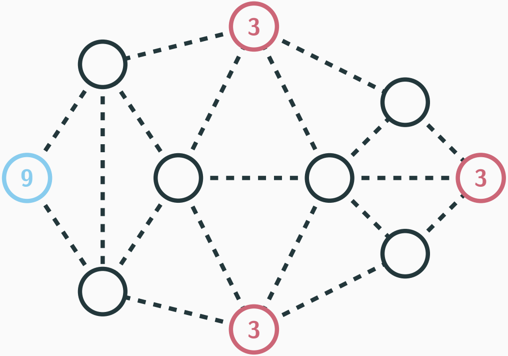
**Model explainability**

Use few features

**Goal**

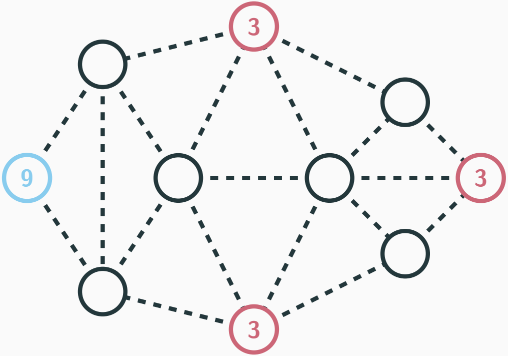
Find $\mathbf{x}$ sparse such that $\mathcal{L}_\phi(\mathbf{A}\mathbf{x}, \mathbf{y})$ is small

# Network design




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

# Network design





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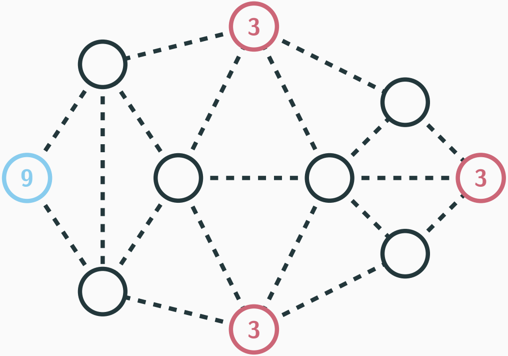


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pay construction cost $c$

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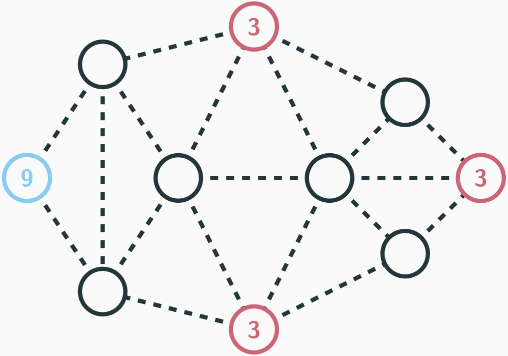


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How to construct the least number of edges to satisfy transportation needs ?

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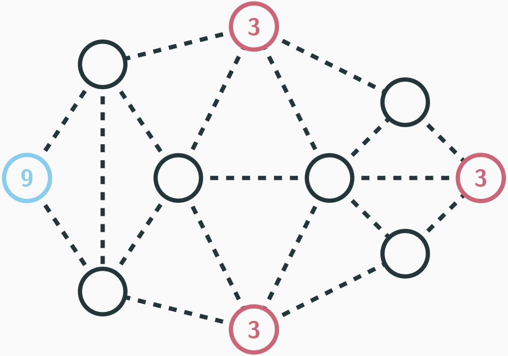


Which edges to build to transport products from source to sink nodes ?


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

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**Question**

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

$\updownarrow$

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

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