

Exact resolution of the sparse spectral unmixing problem

Application of branch-and-bound algorithm

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July 6, 2022



2015 - 2018 Bachelor's degree in computer science and mathematics (Université de Nantes).

2018 - 2020 Master's degree in computer science (Université de Nantes & Université Libre de Bruxelles);
Major in Optimization in Operations Research;
Master's thesis : Branch-and-bound design for ℓ_0 -norm optimization, application to the spectral unmixing problem;
Advisors : S.Bourguignon, R.Ben Mhenni

2020 - 2021 Project engineer (LS2N): algorithm implementation and scientific article redaction.

2021 - 2024 PhD student : Tomographic image reconstruction for a new uncommon 3-photons imaging system (CHU, Centrale Nantes, LS2N);
Advisors : Simon Stute, Jérôme Idier & Thomas Carlier

- ① Assumption, model and definitions
- ② Branch-and-bound algorithm for non-OR community
- ③ Mathematical development and dedicated branch-and-bound
- ④ Some experiments and results
- ⑤ Conclusion

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- 5 Conclusion

Hyperspectral imaging

Let us consider a scene,

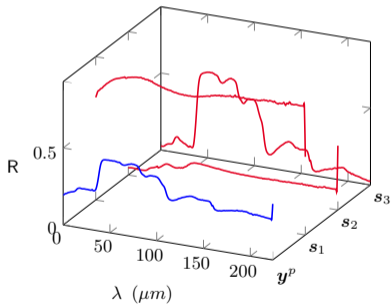
- Extracts information about the **present electromagnetic spectra** over a **large range of spectral bands**;
- A pixel \Rightarrow the observed reflectance spectrum is a **mixture** formed by **different contributions** of the materials **spectral signatures**.

Spectral unmixing problem (SU)

- A **blind source separation** problem i.e. estimate both **spectral signatures** - aka. *atoms* or *endmembers* - and **their proportions** aka. *abundances*;
- **Supervised SU** : the mixture is searched in a known **dictionary** of reference spectra.

Assumption : Linear Mixing Model (LMM)

The **observed mixture** for a pixel can be expressed as the **linear combination of endmembers weighted by the fractional abundances** of each atom.



⇒ For a given pixel observed on N_λ spectral bands :

$$\mathbf{y} = \mathbf{S} \mathbf{a} + \boldsymbol{\varepsilon} \Leftrightarrow \mathbf{y} = \sum_{q \in \llbracket 1, Q \rrbracket} a_q \mathbf{s}_q + \boldsymbol{\varepsilon}$$

where

$\mathbf{y} \in \mathbb{R}^{N_\lambda}$: the reflectance spectrum;

$\mathbf{S} \in \mathbb{R}^{N_\lambda \times Q}$: the dictionary of Q atoms;

$\mathbf{a} \in \mathbb{R}^Q$: the abundance vector;

$\boldsymbol{\varepsilon} \in \mathbb{R}^{N_\lambda}$: additional noise vector;

\mathbf{s}_q, a_q : the q -th atom and its abundance.

$$\mathbf{y} = \sum_{q \in \llbracket 1, Q \rrbracket} a_q \mathbf{s}_q + \boldsymbol{\varepsilon} \quad (\text{LMM})$$

Motivation :

- To express these abundances \mathbf{a} as percentages;
- An active endmember \Rightarrow a nonnegative explanatory contribution to the observed spectrum;
- The reflectance spectrum is only a part of the emitted light (absorption by materials) \sim Normalization of the observed abundances.

Abundance nonnegativity constraint

$$\mathbf{a} \geq 0 \iff a_q \geq 0 \quad \forall q \in \llbracket 1, Q \rrbracket$$

Abundance sum-to-one constraint

$$\mathbf{1}_Q^\top \mathbf{a} = 1 \iff \sum_{q \in \llbracket 1, Q \rrbracket} a_q = 1$$

Remark :

- This SU formulation is well identified in the literature as **Fully Constrained Least Squares** problems [Heinz et al., 2001] which naturally produce solutions where **some abundances are zero**.
- in **complex problems**, the estimated abundances are **spread over a substantial number** of components.

Motivations

- **Physical constraint** : the observed scene is composed of a **limited number** of materials;
- The FCLS formulation may **fail in locating** the true endmembers;
- **Enforcing the number of nonzero abundances** may merely **ensure a correct mixture interpretation**.

The support of \mathbf{a}

$$\text{supp}(\mathbf{a}) := \{q \in \llbracket 1, Q \rrbracket \mid a_q \neq 0\}$$

The counting function : the ℓ_0 -norm

$$\|\mathbf{a}\|_0 := \text{Card}(\text{supp}(\mathbf{a}))$$

K -sparse solution

$$\mathbf{a} \in \mathbb{R}^Q \text{ s.t. } \|\mathbf{a}\|_0 \leq K, \quad K \in \mathbb{Z}_+^*$$

Sparse spectral unmixing problem (ℓ_0 -SU)

$$\begin{aligned} \min_{\mathbf{a} \in [0,1]^Q} \quad & \frac{1}{2} \|\mathbf{y} - \mathbf{S} \mathbf{a}\|_2^2 \\ \text{s.t.} \quad & \|\mathbf{a}\|_0 \leq K, \quad \mathbf{1}_Q^\top \mathbf{a} = 1 \end{aligned} \tag{\mathcal{P}_{2/0}}$$

where $K \in \mathbb{Z}_+^*$ the sparsity coefficient **set a priori**.

It's a complex problem

- ℓ_0 -**"norm"** is not differentiable, not continuous $\Rightarrow \mathcal{P}_{2/0}$ is **not convex**;
- ℓ_0 -**"norm"** minimization problems are \mathcal{NP} -Hard [Natarajan, 1995];
- Can be **only considered** for problems with a **limited amount of atoms**.

But in practice

- The **number of active atoms** in a mixture is relatively **small** e.g. $K \in \llbracket 1, 6 \rrbracket$;
- The **dictionary** is typically composed of $10 \sim 500$ spectral signatures;
- The **sum-to-one & nonnegativity constraints** restrict the space of feasible solutions.

A short state of the art

Approximation: greedy algorithms using heuristics, convex or nonconvex relaxation [Tropp and Wright, 2010]

- **Reduce** the complexity of an **exhaustive exploration**;
- **Rapidly** provide sparse solution;
- The obtained results are **often suboptimal**.

Standard ℓ_0 problems using MIP techniques:

[Bourguignon et al., 2016], [Bertsimas et al., 2016];

Dedicated branch-and-bound algorithm to tackle ℓ_0 problems:

[Bienstock, 1999],[Bertsimas and Shioda, 2009], [Ben Mhenni, 2020], [Hazimeh et al., 2021];

Our approach

Implementing an **exact optimization algorithm** for the ℓ_0 -SU

$$\begin{aligned} \min_{\mathbf{a} \in [0,1]^Q} \quad & \frac{1}{2} \|\mathbf{y} - \mathbf{S} \mathbf{a}\|_2^2 \\ \text{s.t.} \quad & \|\mathbf{a}\|_0 \leq K, \quad \mathbf{1}_Q^\top \mathbf{a} = 1 \end{aligned} \tag{\mathcal{P}_{2/0}}$$

MIP formulation

Introduce a binary decision variables: $\mathbf{b} \in \{0,1\}^Q$ s.t. $a_q = 0 \Leftrightarrow b_q = 0 \quad \forall q \in \llbracket 1, Q \rrbracket$;

Link \mathbf{a} and \mathbf{b} : $|\mathbf{a}| \leq M \mathbf{b}$ with $M \in \mathbb{R}_+^*$ aka. *bigM assumption*;

Trivially with $\mathbf{a} \in [0,1]$: $M = 1$ and $\mathbf{a} \leq \mathbf{b}$

Rewrite the ℓ_0 -norm: $\|\mathbf{a}\|_0 = \sum_{q \in \llbracket 1, Q \rrbracket} b_q$

$$\begin{aligned} \min_{\substack{\mathbf{a} \in [0,1]^Q \\ \mathbf{b} \in \{0,1\}^Q}} \quad & \frac{1}{2} \|\mathbf{y} - \mathbf{S} \mathbf{a}\|_2^2 \\ \text{s.t.} \quad & \sum_{q \in \llbracket 1, Q \rrbracket} b_q \leq K, \quad \mathbf{1}_Q^\top \mathbf{a} = 1, \quad \mathbf{a} \leq \mathbf{b} \end{aligned} \tag{\mathcal{P}_{2/0}}$$

⇒ Just use IBM Cplex solver ...

Our approach

- Implementing a **dedicated** and **exact optimization algorithm** for the ℓ_0 -SU
⇒ Branch-and-bound algorithm;
- Try to be *harder*, *better*, *faster*, *stronger* than a commercial solver [Ben Mhenni, 2020];
- Provide an **open-source** software to the SU community.

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OR's Mantra

When an exhaustive search of all feasible solutions is inconceivable, take a break and implement a branch-and-bound.

Main principle

- Divide & conquer approach;
- Use of bounds on the optimal value to avoid the exploration of some regions of the search space; for a minimization problem :

$$\underline{z} \leq z^* \leq \bar{z}$$

The dual bound $\underline{z} \in \mathbb{R}$: a **lower bound** computed by a **relaxation**, often **easier to compute**;

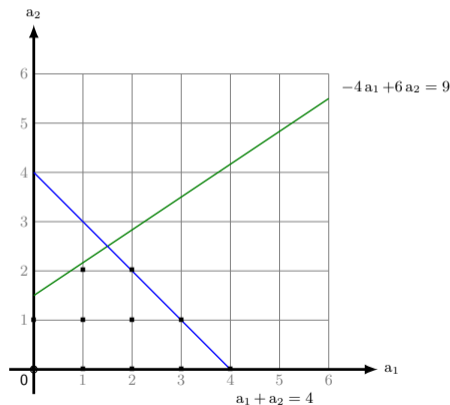
The primal bound $\bar{z} \in \mathbb{R}$: an **upper bound** given by any **feasible** solution.

- Build an **exploration tree** by repeating two steps: the **Branch** & the **Bound** operations.

Branch-and-bound algorithm by the example

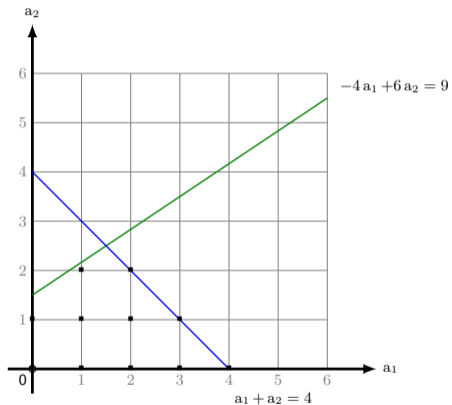
Let us consider:

$$(\mathcal{P}) : \min \{ f(\mathbf{a}) = a_1 - 2a_2 \mid -4a_1 + 6a_2 \leq 9; a_1 + a_2 \leq 4; \mathbf{a} \in \mathbb{Z}_+^2 \}$$



Our objective : find $\hat{\mathbf{a}} := \text{Argmin}(\mathcal{P})$

Branch-and-bound algorithm by the example

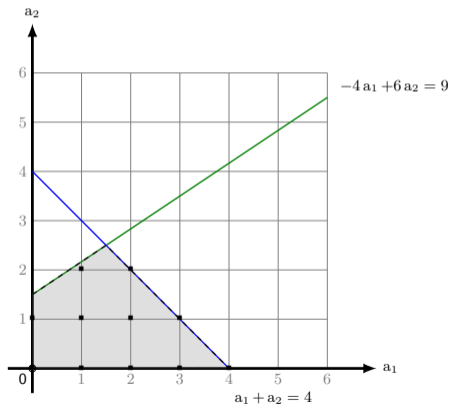


\mathcal{P}_1

$$f(\hat{\mathbf{a}}) = \infty$$

Branch-and-bound algorithm by the example

$$(\mathcal{P}_1) : \min \{ f(\mathbf{a}) = a_1 - 2a_2 \mid -4a_1 + 6a_2 \leq 9; a_1 + a_2 \leq 4; \mathbf{a} \in \mathbb{R}_+^2 \}$$

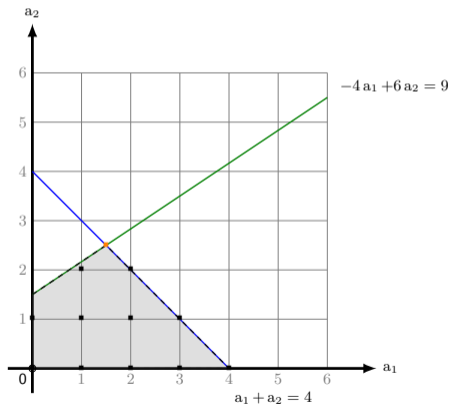


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Branch-and-bound algorithm by the example

$$(\mathcal{P}_1) : \min \{ f(\mathbf{a}) = a_1 - 2a_2 \mid -4a_1 + 6a_2 \leq 9; a_1 + a_2 \leq 4; \mathbf{a} \in \mathbb{R}_+^2 \}$$



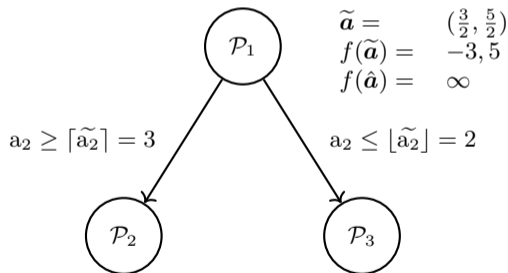
\mathcal{P}_1

$$\begin{aligned} \tilde{\mathbf{a}} &= \left(\frac{3}{2}, \frac{5}{2} \right) \\ f(\tilde{\mathbf{a}}) &= -3,5 \\ f(\hat{\mathbf{a}}) &= \infty \end{aligned}$$

Branch-and-bound algorithm by the example

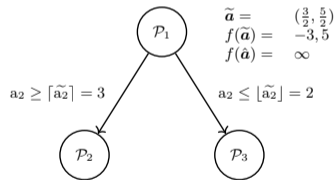
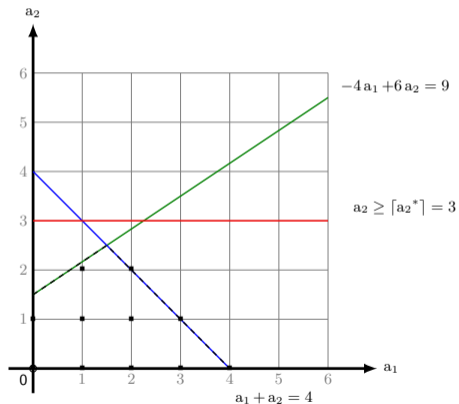
Branch : Use the optimum value to define inequalities and create a b -partition of the search space (exhaustive but not necessarily mutually exclusive);

e.g. Most infeasible branching \Leftrightarrow most fractional component



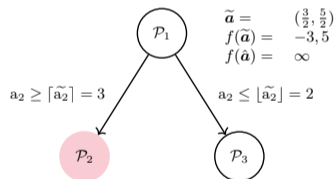
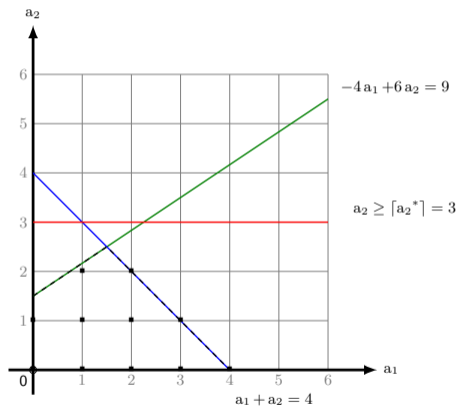
Branch-and-bound algorithm by the example

$$\mathcal{P}_2 := \mathcal{P}_1 \cap \{a_2 \geq 3\}$$



Branch-and-bound algorithm by the example

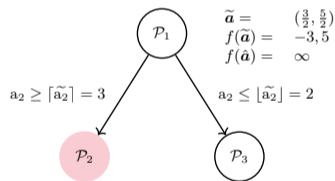
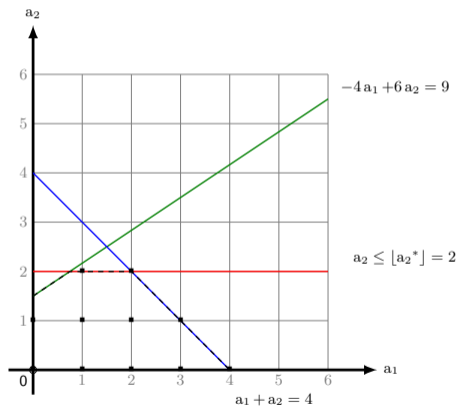
$$\mathcal{P}_2 := \mathcal{P}_1 \cap \{a_2 \geq 3\}$$



⇒ Pruning \mathcal{P}_2 by **nonfeasibility** !

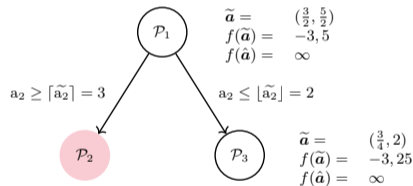
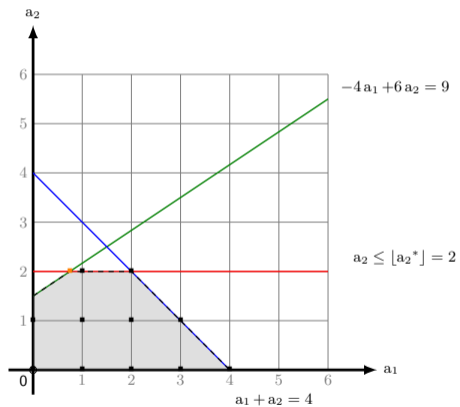
Branch-and-bound algorithm by the example

$$\mathcal{P}_3 := \mathcal{P}_1 \cap \{a_2 \leq 2\}$$



Branch-and-bound algorithm by the example

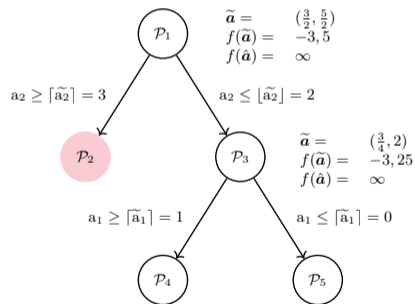
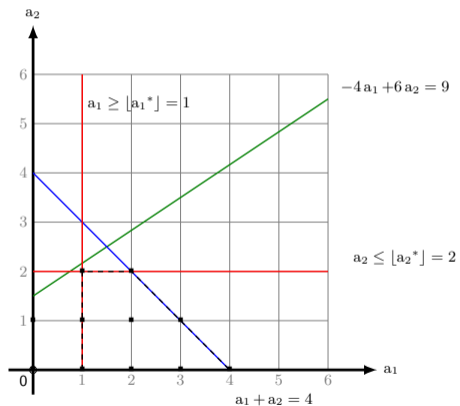
$$\mathcal{P}_3 := \mathcal{P}_1 \cap \{a_2 \leq 2\}$$



⇒ Nothing can be concluded: **Branch** on \mathcal{P}_3 !

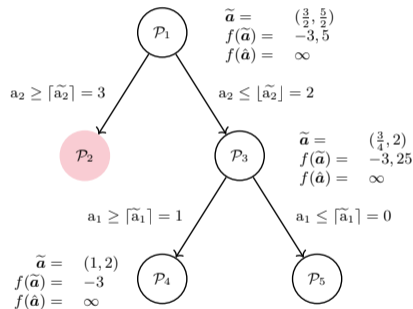
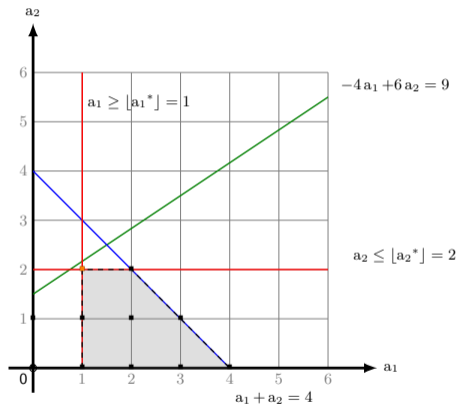
Branch-and-bound algorithm by the example

$$\mathcal{P}_4 := \mathcal{P}_1 \cap \{a_2 \leq 2\} \cap \{a_1 \geq 1\}$$



Branch-and-bound algorithm by the example

$$\mathcal{P}_4 := \mathcal{P}_1 \cap \{a_2 \leq 2\} \cap \{a_1 \geq 1\}$$

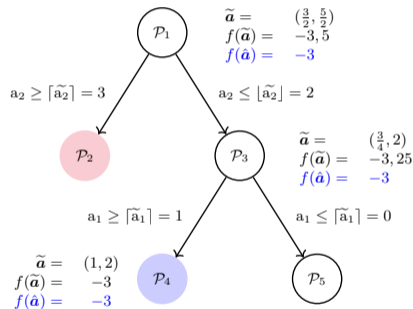
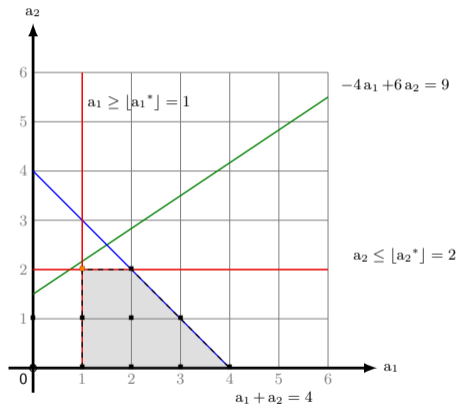


⇒ Prune \mathcal{P}_4 by **optimality** i.e. $\exists \tilde{\mathbf{a}} \in \mathbb{Z}_+$ -feasible s.t. $f(\tilde{\mathbf{a}}) < f(\hat{\mathbf{a}})$;

⇒ Update the global upper bound $f(\hat{\mathbf{a}})$

Branch-and-bound algorithm by the example

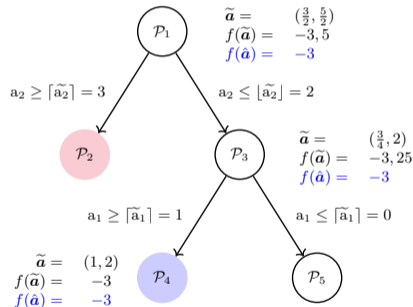
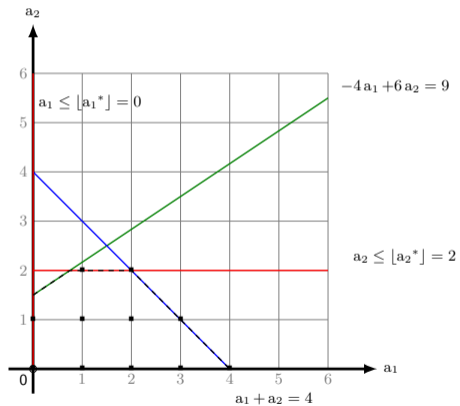
$$\mathcal{P}_4 := \mathcal{P}_1 \cap \{a_2 \leq 2\} \cap \{a_1 \geq 1\}$$



- ⇒ Prune \mathcal{P}_4 by **optimality** i.e. $\exists \tilde{\mathbf{a}} \in \mathbb{Z}_+$ -feasible s.t. $f(\tilde{\mathbf{a}}) < f(\hat{\mathbf{a}})$;
- ⇒ Update the global upper bound $f(\hat{\mathbf{a}})$

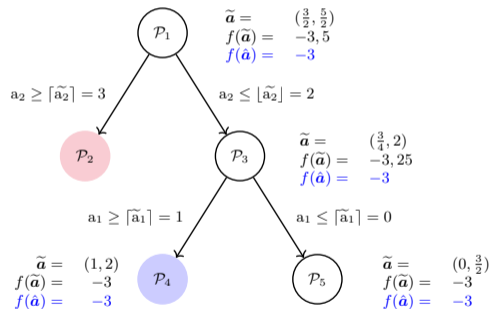
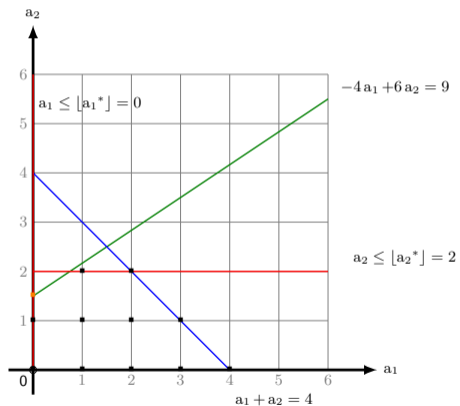
Branch-and-bound algorithm by the example

$$\mathcal{P}_5 := \mathcal{P}_1 \cap \{a_2 \leq 2\} \cap \{a_1 \leq 0\}$$



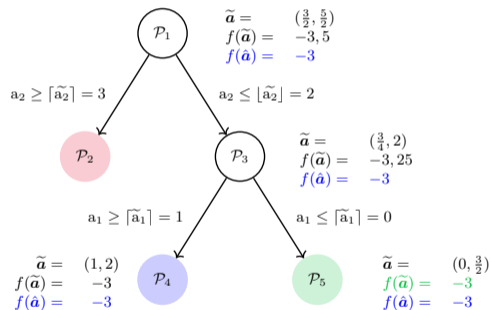
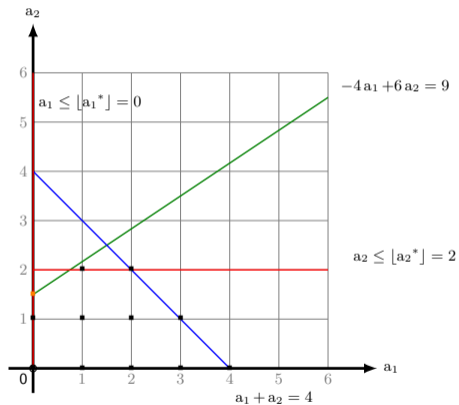
Branch-and-bound algorithm by the example

$$\mathcal{P}_5 := \mathcal{P}_1 \cap \{a_2 \leq 2\} \cap \{a_1 \leq 0\}$$



Branch-and-bound algorithm by the example

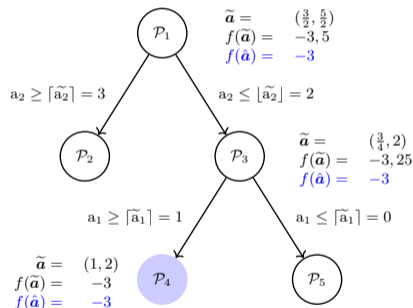
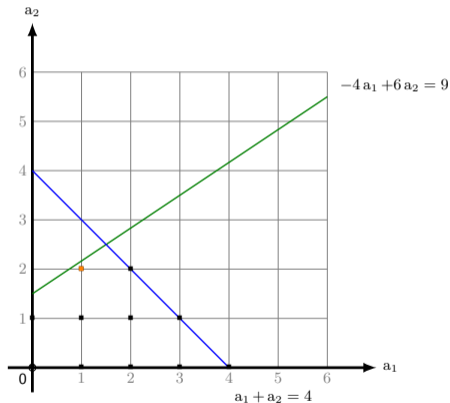
$$\mathcal{P}_5 := \mathcal{P}_1 \cap \{a_2 \leq 2\} \cap \{a_1 \leq 0\}$$



⇒ Prune \mathcal{P}_5 by **dominance** i.e. $\forall \tilde{\mathbf{a}}, f(\tilde{\mathbf{a}}) \geq f(\hat{\mathbf{a}})$;

Branch-and-bound algorithm by the example

$$(\mathcal{P}) : \min \{ f(\mathbf{a}) = a_1 - 2a_2 \mid -4a_1 + 6a_2 \leq 9; a_1 + a_2 \leq 4; \mathbf{a} \in \mathbb{Z}_+^2 \}$$



\Rightarrow **Founded and certified optimality** : $\hat{\mathbf{a}} = (1, 2)$, $f(\hat{\mathbf{a}}) = -3$.

Computational complexity: $\mathcal{O}(Tb^Q)$ with

b : *branching factor*

T : a fixed bound on time needed to explore the search (sub)spaces;

Q : the length of the longest path from the root to a leaf.

How to tune this algorithm ?

Branching strategy:

- Which value for the $b \in \mathbb{N}^*$?
- How to choose the branching variable a_i ?

Pruning rules:

- How to compute the lower bounds ?
- Add other valid inequality, cutting planes, dominance rules, ...

Search strategy:

- How to explore the tree ? e.g. DFS, BFS, ...

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$$\min_{\mathbf{a} \in [0,1]^Q} \frac{1}{2} \|\mathbf{y} - \mathbf{S} \mathbf{a}\|_2^2 \quad \text{s.t.} \quad \|\mathbf{a}\|_0 \leq K, \quad \mathbf{1}_Q^\top \mathbf{a} = 1 \quad (\mathcal{P}_{2/0})$$

The branch-and-bound will solve many subproblems on different subspaces :

Set notations

Let $\mathbb{S} := \llbracket 1, Q \rrbracket$,

The discarded variables: $\mathcal{Z} := \{q \in \mathbb{S} \mid a_q \notin \text{supp}(\mathbf{a})\} \subset \mathbb{S}$;

The remaining variables on $[0, 1]$: $\bar{\mathcal{Z}} := \mathbb{S} \setminus \mathcal{Z}$ with $\bar{n} := \mathbf{Card}(\bar{\mathcal{Z}})$

The chosen variables: $\mathcal{C} \subset \bar{\mathcal{Z}}$

The **general formulation** of the subproblems :

$$\min_{\mathbf{a}_{\bar{\mathcal{Z}}} \in [0,1]^{\bar{n}}} \frac{1}{2} \|\mathbf{y} - \mathbf{S}_{\bar{\mathcal{Z}}} \mathbf{a}_{\bar{\mathcal{Z}}}\|_2^2 \quad \text{s.t.} \quad \|\mathbf{a}_{\bar{\mathcal{Z}}}\|_0 \leq \hat{K} - \mathbf{Card}(\mathcal{C}), \quad \mathbf{1}_{\bar{\mathcal{Z}}}^\top \mathbf{a}_{\bar{\mathcal{Z}}} = 1 \quad (\mathcal{P}_{2/0})$$

ℓ_0 -norm convex relaxation:

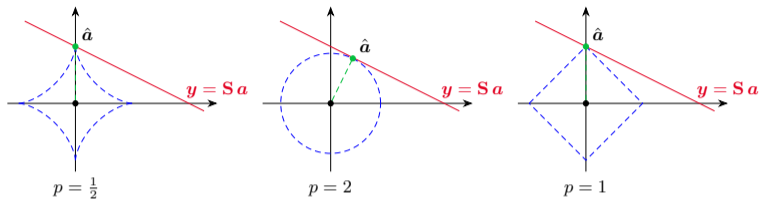


Figure: ℓ_p -norm $\forall p \in \{\frac{1}{2}, 2, 1\}$

Which one to choose?

Constraint : preserve the sparsity of the solutions;

- ℓ_p -norm with $p \in]0, 1[$: sparse solution **but nonconvex** norm **and** we need to **ensure the optimality** of the solution
- ℓ_2 -norm: **nonsparse** solution **but** convex norm;
- ℓ_1 -norm: sparse solution **and** convex norm;

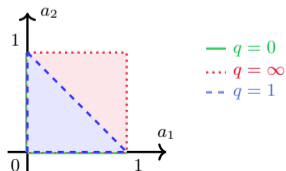
ℓ_0 -norm convex relaxation:

$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \|\mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}}\|_2^2 \quad \text{s.t.} \quad \|\mathbf{a}_{\bar{z}}\|_0 \leq K - \text{Card}(\mathcal{C}), \quad \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/0})$$

Rewrite the sparsity constraint:

Using $\mathcal{B}_p^K := \{ \mathbf{a} \in \mathbb{R}^Q \mid \|\mathbf{a}\|_p \leq K \}$, $K \in \mathbb{Z}_+^*$: $\mathbf{a} \in ([0,1]^{\bar{n}} \cap \mathcal{B}_0^{K - \text{Card}(\mathcal{C})})$

$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \|\mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}}\|_2^2 \quad \text{s.t.} \quad \mathbf{a}_{\bar{z}} \in \mathcal{B}_0^{K - \text{Card}(\mathcal{C})}, \quad \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/0})$$



Property : the ℓ_1 relaxation

Given $K \in \mathbb{N}^*$ and under bound constraints:

$$\text{conv}([0,1]^Q \cap \mathcal{B}_0^K) = ([0,1]^Q \cap \mathcal{B}_1^K)$$

ℓ_0 -norm convex relaxation:

$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \left\| \mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}} \right\|_2^2 \quad \text{s.t.} \quad \mathbf{a}_{\bar{z}} \in \mathcal{B}_0^{K - \text{Card}(\mathcal{C})}, \quad \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/0})$$

$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \left\| \mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}} \right\|_2^2 \quad \text{s.t.} \quad \mathbf{a}_{\bar{z}} \in \mathcal{B}_1^{K - \text{Card}(\mathcal{C})}, \quad \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/1})$$

Beware of sparsity constraint !!

When $K > \text{Card}(\mathcal{C})$, the relaxed sparsity constraint is **dominated** by the sum-to-one constraint; it can be **withdrawn** of $\mathcal{P}_{2/1}$.

$$\rightsquigarrow \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} \leq K - \text{Card}(\mathcal{C}) \wedge K > \text{Card}(\mathcal{C}) \implies K - \text{Card}(\mathcal{C}) > 1 \wedge \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} \leq 1$$

$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \left\| \mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}} \right\|_2^2 \quad \text{s.t.} \quad \mathbf{a}_{\bar{z}} \in \mathcal{B}_1^{K - \text{Card}(\mathcal{C})}, \quad \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/1})$$

\Rightarrow Just another FCLS formulation.

Branching procedure - $K > \text{Card}(\mathcal{C})$

ℓ_0 -**"norm"** subproblem:

$$\min_{\mathbf{a}_{\bar{Z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \left\| \mathbf{y} - \mathbf{S}_{\bar{Z}} \mathbf{a}_{\bar{Z}} \right\|_2^2 \quad \text{s.t.} \quad \mathbf{a}_{\bar{Z}} \in \mathcal{B}_0^{K - \text{Card}(\mathcal{C})}, \quad \mathbf{1}_{\bar{Z}}^\top \mathbf{a}_{\bar{Z}} = 1 \quad (\mathcal{P}_{2/0})$$

ℓ_1 -**"norm"** subproblem:

$$\min_{\mathbf{a}_{\bar{Z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \left\| \mathbf{y} - \mathbf{S}_{\bar{Z}} \mathbf{a}_{\bar{Z}} \right\|_2^2 \quad \text{s.t.} \quad \mathbf{1}_{\bar{Z}}^\top \mathbf{a}_{\bar{Z}} = 1 \quad (\mathcal{P}_{2/1})$$

Main idea

To select an atom to add in the support of $\mathcal{P}_{2/0}$:

- Compute $\hat{\mathbf{a}} := \text{Argmin}(\mathcal{P}_{2/1})$
- Choose the q -th endmember

$$q := \text{argmax}_{i \in \bar{Z} \setminus \mathcal{C}} (\hat{a}_i)$$

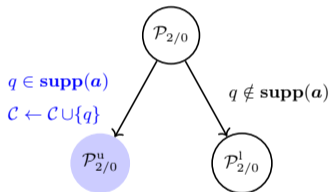
- Apply a binary branching strategy on the q -th endmember, i.e. $\forall q \in \bar{Z} \setminus \mathcal{C}$

$$q \in \text{supp}(\mathbf{a}) \quad \text{or} \quad q \notin \text{supp}(\mathbf{a})$$

Branching procedure - $K > \text{Card}(\mathcal{C}) - q \in \text{supp}(\mathbf{a})$

$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \|\mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}}\|_2^2 \quad \text{s.t.} \quad \mathbf{a}_{\bar{z}} \in \mathcal{B}_0^{K - \text{Card}(\mathcal{C})}, \quad \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/0})$$

$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \|\mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}}\|_2^2 \quad \text{s.t.} \quad \mathbf{1}_{\bar{z}}^\top \hat{\mathbf{a}}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/1})$$



$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \|\mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}}\|_2^2 \quad \text{s.t.} \quad \mathbf{a}_{\bar{z}} \in \mathcal{B}_0^{K - (\text{Card}(\mathcal{C})+1)}, \quad \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/0}^u)$$

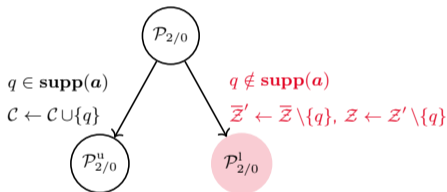
$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \|\mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}}\|_2^2 \quad \text{s.t.} \quad \mathbf{1}_{\bar{z}}^\top \hat{\mathbf{a}}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/1}^u)$$

⇒ Same relaxations, **Nothing to do.**

Branching procedure - $K > \text{Card}(\mathcal{C}) - q \notin \text{supp}(\mathbf{a})$

$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \left\| \mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}} \right\|_2^2 \quad \text{s.t.} \quad \mathbf{a}_{\bar{z}} \in \mathcal{B}_0^{K - \text{Card}(\mathcal{C})}, \quad \mathbf{1}_{\bar{z}}^\top \mathbf{a}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/0})$$

$$\min_{\mathbf{a}_{\bar{z}} \in [0,1]^{\bar{n}}} \frac{1}{2} \left\| \mathbf{y} - \mathbf{S}_{\bar{z}} \mathbf{a}_{\bar{z}} \right\|_2^2 \quad \text{s.t.} \quad \mathbf{1}_{\bar{z}}^\top \hat{\mathbf{a}}_{\bar{z}} = 1 \quad (\mathcal{P}_{2/1})$$



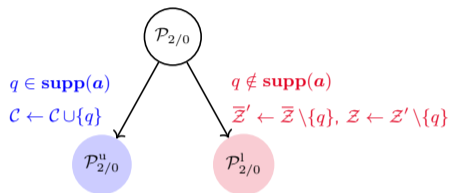
$$\min_{\mathbf{a}_{\bar{z}'} \in [0,1]^{\bar{n}'}} \frac{1}{2} \left\| \mathbf{y} - \mathbf{S}_{\bar{z}'} \mathbf{a}_{\bar{z}'} \right\|_2^2 \quad \text{s.t.} \quad \mathbf{a}_{\bar{z}'} \in \mathcal{B}_0^{K - \text{Card}(\mathcal{C})}, \quad \mathbf{1}_{\bar{z}'}^\top \mathbf{a}_{\bar{z}'} = 1 \quad (\mathcal{P}_{2/0}^l)$$

$$\min_{\mathbf{a}_{\bar{z}'} \in [0,1]^{\bar{n}'}} \frac{1}{2} \left\| \mathbf{y} - \mathbf{S}_{\bar{z}'} \mathbf{a}_{\bar{z}'} \right\|_2^2 \quad \text{s.t.} \quad \mathbf{1}_{\bar{z}'}^\top \mathbf{a}_{\bar{z}'} = 1 \quad (\mathcal{P}_{2/1}^l)$$

⇒ Different relaxations, **A new FCLS problem.**

Branching procedure - $K = \text{Card}(\mathcal{C})$

Additional assumption: $\hat{a} := \text{Argmin}(\mathcal{P}_{2/1})$ and $\|\hat{a}\|_0 = K - 1$



$$\min_{\mathbf{a}_C \in [0,1]^K} \frac{1}{2} \|\mathbf{y} - \mathbf{S}_C \mathbf{a}_C\|_2^2 \quad \text{s.t.} \quad \mathbf{1}_C^\top \mathbf{a}_C = 1 \quad (\mathcal{P}_{2/1}^u)$$

$$\min_{\mathbf{a}_{\bar{Z}'} \in [0,1]^{\bar{n}'}} \frac{1}{2} \|\mathbf{y} - \mathbf{S}_{\bar{Z}'} \mathbf{a}_{\bar{Z}'}\|_2^2 \quad \text{s.t.} \quad \mathbf{1}_{\bar{Z}'}^\top \mathbf{a}_{\bar{Z}'} = 1 \quad (\mathcal{P}_{2/1}^l)$$

$\mathcal{P}_{2/1}^l$: to gather the best subset of atoms in the search subspace and get **feasible nonsparse solutions** i.e. **lower** bounds;

$\mathcal{P}_{2/1}^u$: to fit the optimal abundances of the selected $\text{supp}(\mathbf{a})$ and get K -sparse **feasible solutions** i.e. **upper** bounds.

The dedicated branch-and-bound

Lower bound evaluations:

- Right child:
⇒ Solve $\mathcal{P}_{2/1}^l$ to get lower bound,
⇒ try to fathomed the node;
- Left child $\wedge K = \text{Card}(\mathcal{C})$:
⇒ Solve $\mathcal{P}_{2/1}^u$ to get upper bound,
⇒ fathomed the node;
- Left child $\wedge K > \text{Card}(\mathcal{C})$:
⇒ Just branch on $q \in \bar{\mathcal{Z}} \setminus \mathcal{C}$.

Search strategy:

DFS: to quickly find \widehat{K} -sparse solutions

Algorithme 1 : Dedicated branch-and-bound algorithm

Data : $\widehat{K}, \mathbb{S}, \mathbf{y}, \mathbb{S}$

Result : $(\hat{\mathbf{a}}, \hat{z})$

Initialization :

1 $\bar{\mathcal{Z}} \leftarrow \mathbb{S}, \mathcal{Z} \leftarrow \emptyset, \mathcal{C} \leftarrow \emptyset, n \leftarrow 0, L \leftarrow \emptyset$

2 $\hat{\mathbf{a}} \leftarrow \mathbf{0}_Q, \hat{z} \leftarrow \|\mathbf{y}\|_2^2$

3 **push** $(L, (\mathcal{C}, \bar{\mathcal{Z}}, \mathcal{Z}, n))$

Main loop :

4 **while** $(L \neq \emptyset)$ **do**

5 $(\mathcal{C}, \bar{\mathcal{Z}}, \mathcal{Z}, n) \leftarrow \text{pop}(L)$

6 **terminal** \leftarrow false

Node evaluation procedure :

7 $(\bar{\mathbf{a}}, \bar{z}) \leftarrow \text{solve}(\mathcal{P}_n^f, \mathcal{C}, \bar{\mathcal{Z}}, \mathcal{Z}) \forall f \in \{u, l, b\}$

Bound procedure :

8 **if** $(\bar{z} \geq \hat{z})$ **then** // Fathomed by dominance

9 | **terminal** \leftarrow true

10 **else if** $(\bar{z} < \hat{z})$ **then** // Fathomed by optimality

11 | **terminal** \leftarrow true, $\hat{\mathbf{a}} \leftarrow \bar{\mathbf{a}}, \hat{z} \leftarrow \bar{z}$

end

Branch procedure :

12 **if** $(\neg \text{terminal} \wedge \text{Card}(\bar{\mathbb{S}}) \neq \emptyset)$ **then**

13 | $q \leftarrow \text{argmax}_{i \in \bar{\mathbb{S}}}(\hat{\mathbf{a}}_i \mid \hat{\mathbf{a}}_i > 0)$

14 | // Insert Right and Left children in L

15 | **push** $(L, (\mathcal{C}, \mathcal{Z} \cup \{q\}, \bar{\mathcal{Z}} \setminus \{q\}, 2n + 2))$

16 | **push** $(L, (\mathcal{C} \cup \{q\}, \mathcal{Z}, \bar{\mathcal{Z}} \setminus \{q\}, 2n + 1))$

end

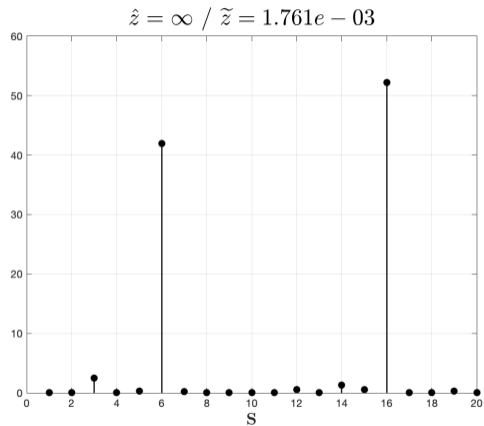
end

The dedicated branch-and-bound: Example with $K = 3$, $Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$

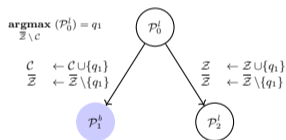
\mathcal{P}_0^l

$\mathcal{C} = \emptyset$

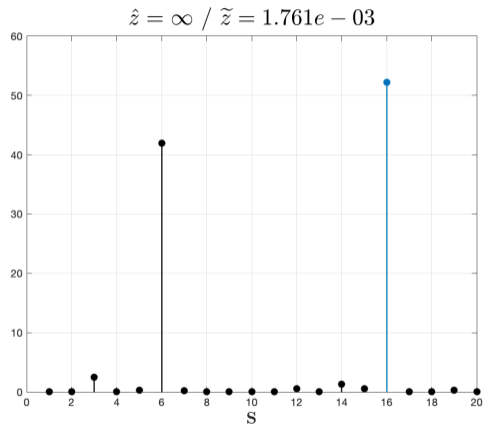


The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$

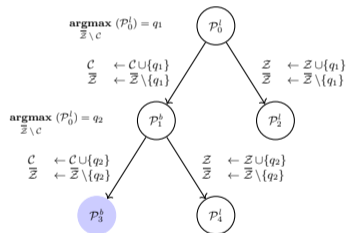


$$\mathcal{C} = \{16\}$$

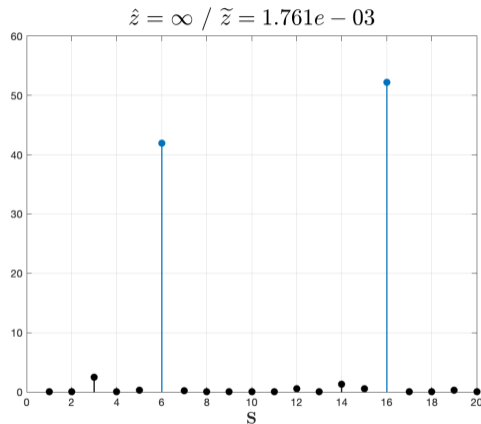


The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$

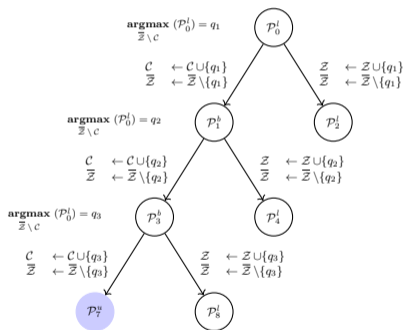


$$C = \{16, 6\}$$

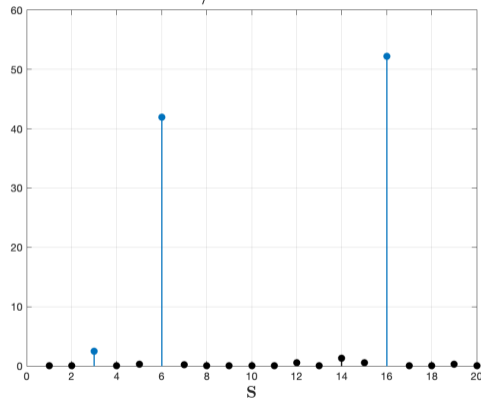


The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$



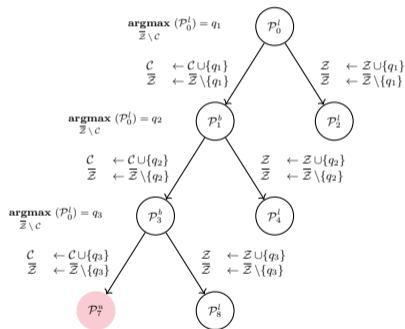
$$\hat{z} = \infty / \tilde{z} = 1.761e - 03$$



$$C = \{16, 6, 3\} \quad \wedge \quad \text{Card}(C) = K$$

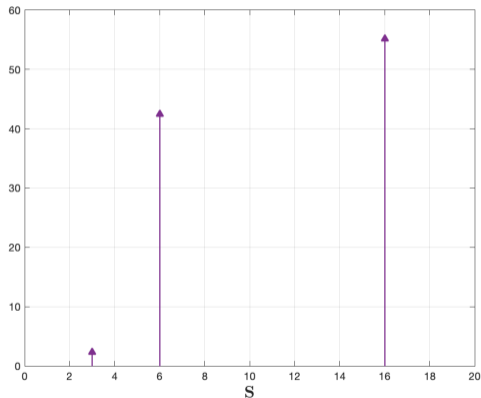
The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$



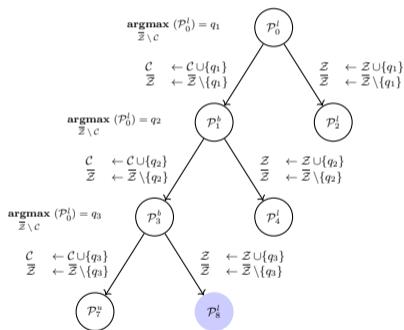
$$C = \{16, 6, 3\}$$

$$\hat{z} = \tilde{z} = 1.789e - 03$$



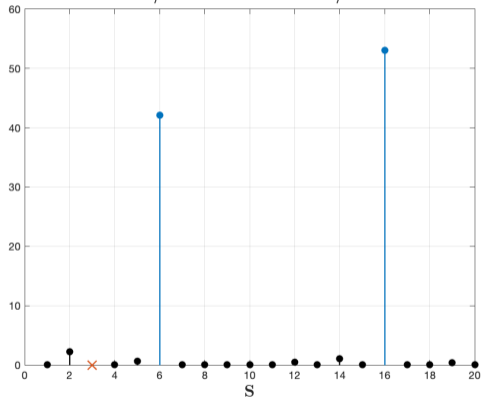
The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$



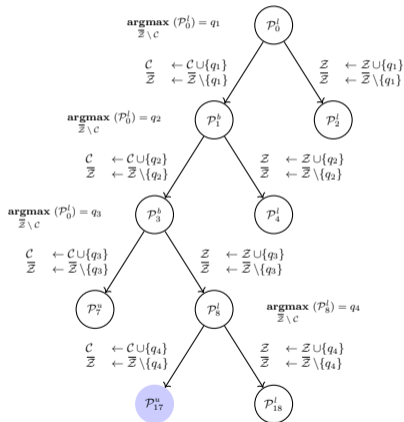
$$C = \{16, 6\}$$

$$\hat{z} = 1.789e - 03 / \tilde{z} = 1.781e - 03 / \delta = 7.948e - 06$$



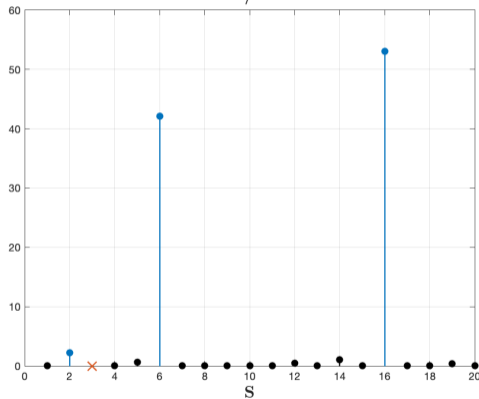
The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$



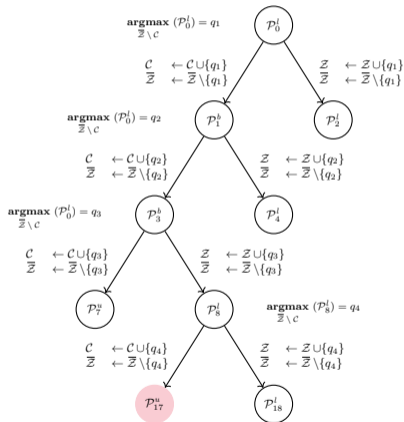
$$C = \{16, 6, 2\} \wedge \text{Card}(C) = K$$

$$\hat{z} = 1.789e - 03 / \tilde{z} = 1.781e - 03$$



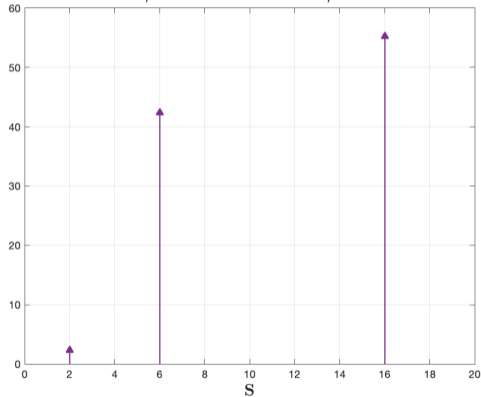
The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$



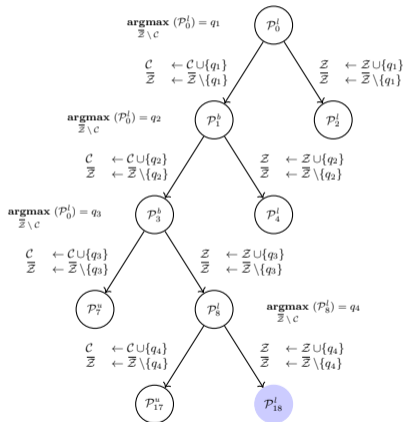
$$C = \{16, 6, 2\}$$

$$\hat{z} = 1.789e - 03 / \tilde{z} = 1.814e - 03 / \delta = -2.500e - 05$$



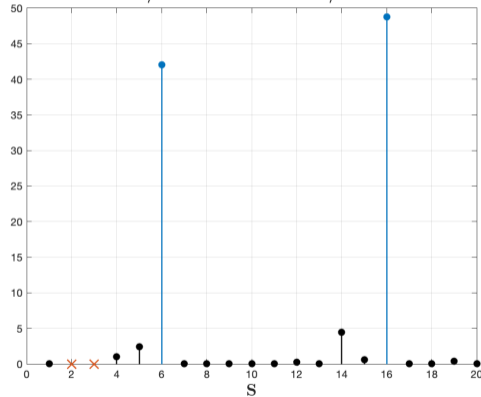
The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$



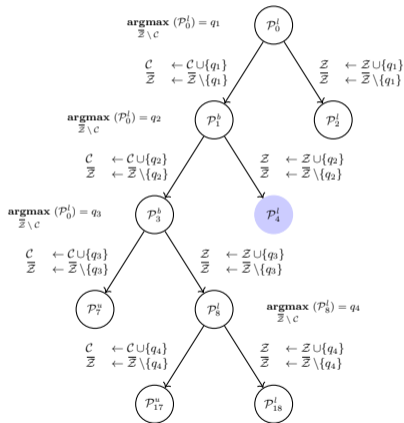
$$C = \{16, 6\}$$

$$\hat{z} = 1.789e - 03 / \tilde{z} = 1.841e - 03 / \delta = -5.203e - 05$$



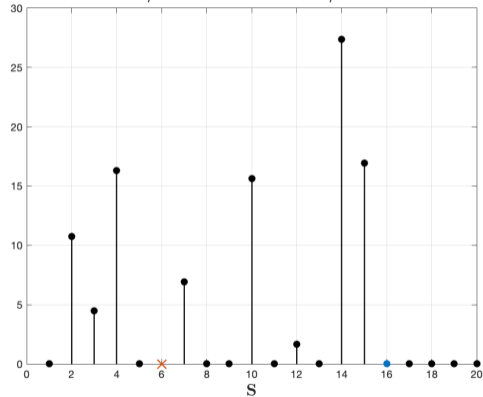
The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$



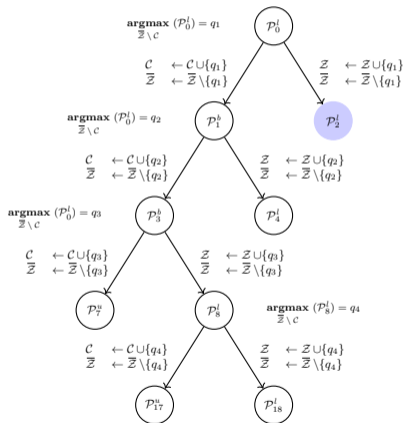
$$C = \{16\}$$

$$\hat{z} = 1.789e - 03 / \tilde{z} = 1.984e - 02 / \delta = -1.805e - 02$$



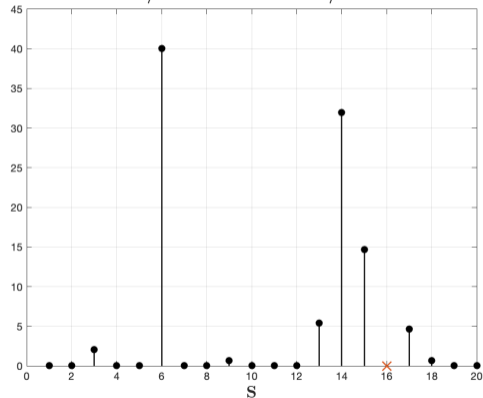
The dedicated branch-and-bound: Example with $K = 3, Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$



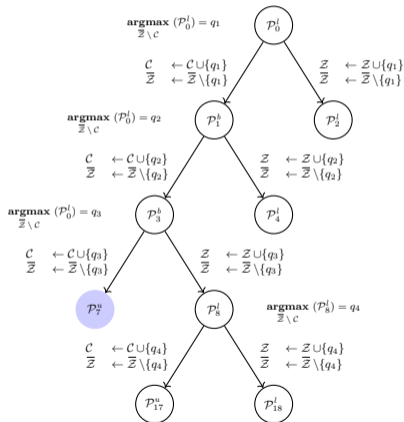
$$C = \emptyset$$

$$\hat{z} = 1.789e - 03 / \tilde{z} = 2.782e - 03 / \delta = -9.931e - 04$$

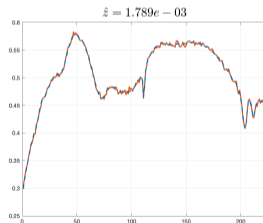
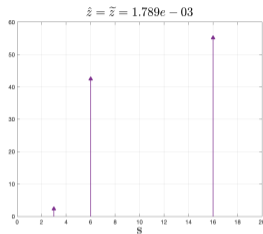


The dedicated branch-and-bound: Example with $K = 3$, $Q = 20$

Notations : \hat{z} the best feasible solution, \tilde{z} the current solution, $\delta = \hat{z} - \tilde{z}$



$$C = \{16, 6, 3\}$$



- ① Assumption, model and definitions
- ② Branch-and-bound algorithm for non-OR community
- ③ Mathematical development and dedicated branch-and-bound
- ④ **Some experiments and results**
- ⑤ Conclusion



Figure: Source : South Park - Season 18 (2014)

USGS Digital Spectral Libraries

- $Q = 498$ pure spectral signatures (Minerals, Vegetation, Manmade materials, ...)
- $N_\lambda = 224$ samples and the wavelength coverage is $[0.3, 2.7] \mu\text{m}$

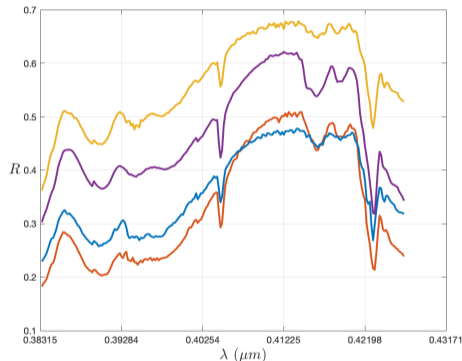


Figure: USGS atoms Calcite : **AMX7**, **AMX18**, **AMX6**, **AMX43**

Instances generation protocol

Two sets of designed problems such as:

Number of atoms: $Q \in \{20, 50, 100, 200, 300, 400, 498\}$;

Sparsity level: $\hat{K} \in \llbracket 2, 6 \rrbracket$;

Some noise: $\text{SNR} \in \{40, 45, 50, 55, 60, \infty\}$ dB;

A minimum threshold: on the abundances $\tau = 0.1$;

Permutations of \mathbf{S} : 20.

Investigated methods

Time comparison:

B&B: our branch-and-bound with qpOASES solver [Ferreau et al., 2014] (C++)

MIP: using IBM Cplex solver (C++)

Quality comparison:

SDA: An iterative deflation algorithm [Greer, 2011] (Matlab)

\hat{K} -FCLS: Two-phase algorithm using IBM Cplex solver (Matlab)

Simulated problems on USGS - Time comparison

SNR = ∞		B&B	MIP	Ratio	SNR = 60dB		B&B	MIP	Ratio
Q = 20	$\hat{K} = 2$	7,59e-04	8,23e-03	0,092	Q = 20	$\hat{K} = 2$	6,46e-04	7,36e-03	0,088
	$\hat{K} = 4$	1,45e-03	6,17e-03	0,234		$\hat{K} = 4$	1,45e-03	8,19e-03	0,177
	$\hat{K} = 6$	2,38e-03	6,70e-03	0,356		$\hat{K} = 6$	2,17e-03	8,17e-03	0,265
Q = 100	$\hat{K} = 2$	1,70e-02	7,63e-02	0,223	Q = 100	$\hat{K} = 2$	5,39e-03	7,61e-02	0,071
	$\hat{K} = 4$	1,86e-02	7,16e-02	0,26		$\hat{K} = 4$	1,47e-02	7,68e-02	0,192
	$\hat{K} = 6$	3,64e-02	7,33e-02	0,497		$\hat{K} = 6$	2,57e-02	1,63e-01	0,158
Q = 498	$\hat{K} = 2$	4,17e-01	6,95	0,06	Q = 498	$\hat{K} = 2$	2,79e-01	2,14	0,131
	$\hat{K} = 4$	1,03	9,28	0,11		$\hat{K} = 4$	2,77	2,99	0,926
	$\hat{K} = 6$	1,93	1,91e+01	0,1		$\hat{K} = 6$	8,97	4,75	1,889

SNR = 50dB		B&B	MIP	Ratio	SNR = 40dB		B&B	MIP	Ratio
Q = 20	$\hat{K} = 2$	5,76e-04	8,97e-03	0,064	Q = 20	$\hat{K} = 2$	6,91e-04	1,40e-02	0,049
	$\hat{K} = 4$	1,15e-03	3,21e-02	0,036		$\hat{K} = 4$	1,37e-03	1,01e-02	0,136
	$\hat{K} = 6$	1,64e-03	9,03e-03	0,182		$\hat{K} = 6$	2,18e-03	9,71e-03	0,225
Q = 100	$\hat{K} = 2$	4,55e-03	9,41e-02	0,048	Q = 100	$\hat{K} = 2$	7,61e-03	1,10e-01	0,069
	$\hat{K} = 4$	1,39e-02	7,67e-02	0,181		$\hat{K} = 4$	5,36e-02	1,35e-01	0,398
	$\hat{K} = 6$	7,49e-02	1,84e-01	0,406		$\hat{K} = 6$	7,35e-01	4,18e-01	1,760
Q = 498	$\hat{K} = 2$	5,29e-01	2,88	0,184	Q = 498	$\hat{K} = 2$	7,95	4,91	1,619
	$\hat{K} = 4$	3,11e+01	1,74e+01	1,789		$\hat{K} = 4$	4,39e+02	2,39e+02	1,834
	$\hat{K} = 6$	3,12e+02	1,51e+02	2,062		$\hat{K} = 6$	9,08e+02	7,52e+02	1,208

- The exact method can be used to solve ℓ_0 -SU problems
- The ratio of execution times seems to be favorable to our dedicated approach, except for the most difficult problems

Simulated problems on USGS - Quality comparison

Metric Exact Recovery Ratio (as %) : $ERR := (\text{supp}(\hat{\mathbf{a}}) \cap \text{supp}(\hat{\mathbf{a}})) / \hat{K}$

SNR = ∞		B&B	SDA	\hat{K} -FCLS
Q = 20	$\hat{K} = 2$	100	100	100
	$\hat{K} = 4$	100	100	100
	$\hat{K} = 6$	100	100	100
Q = 100	$\hat{K} = 2$	100	100	100
	$\hat{K} = 4$	100	100	100
	$\hat{K} = 6$	100	100	100
Q = 498	$\hat{K} = 2$	100	100	100
	$\hat{K} = 4$	100	100	100
	$\hat{K} = 6$	100	100	100

SNR = 60dB		B&B	SDA	\hat{K} -FCLS
Q = 20	$\hat{K} = 2$	100,0	100,0	100,0
	$\hat{K} = 4$	100,0	100,0	100,0
	$\hat{K} = 6$	100,0	100,0	100,0
Q = 100	$\hat{K} = 2$	100,0	100,0	100,0
	$\hat{K} = 4$	100,0	100,0	100,0
	$\hat{K} = 6$	100,0	100,0	99,2
Q = 498	$\hat{K} = 2$	100,0	100,0	100,0
	$\hat{K} = 4$	100,0	100,0	100,0
	$\hat{K} = 6$	100,0	99,6	98,3

SNR = 50dB		B&B	SDA	\hat{K} -FCLS
Q = 20	$\hat{K} = 2$	100,0	100,0	100,0
	$\hat{K} = 4$	100,0	100,0	100,0
	$\hat{K} = 6$	100,0	100,0	100,0
Q = 100	$\hat{K} = 2$	100,0	100,0	100,0
	$\hat{K} = 4$	100,0	100,0	100,0
	$\hat{K} = 6$	100,0	99,6	97,9
Q = 498	$\hat{K} = 2$	100,0	98,8	97,5
	$\hat{K} = 4$	100,0	98,1	91,9
	$\hat{K} = 6$	97,1	91,7	89,6

SNR = 40dB		B&B	SDA	\hat{K} -FCLS
Q = 20	$\hat{K} = 2$	100,0	100,0	100,0
	$\hat{K} = 4$	100,0	100,0	100,0
	$\hat{K} = 6$	98,8	99,2	97,1
Q = 100	$\hat{K} = 2$	100,0	98,8	97,5
	$\hat{K} = 4$	100,0	94,4	92,5
	$\hat{K} = 6$	95,0	92,1	87,9
Q = 498	$\hat{K} = 2$	100,0	93,8	86,3
	$\hat{K} = 4$	85,6	76,9	65,0
	$\hat{K} = 6$	63,8	55,0	52,1

- Giving time to exactly solve the ℓ_0 -SU is quite interesting !

- ① Assumption, model and definitions
- ② Branch-and-bound algorithm for non-OR community
- ③ Mathematical development and dedicated branch-and-bound
- ④ Some experiments and results
- ⑤ Conclusion

To work with (semi)real datasets: Collaboration with Lucas Drumetz (IMT Atlantique)

- **Unsupervised SU**;
- The dictionary, composed of $Q = 15$ spectra, is learned from a data set;
- **Teaser**
 - Branch-and-bound algorithm is **very promising** in regards to **computation time**;
 - We are in a position to show **the interest of exact optimization**;
 - We have some problems with the **interpretability** of the data in the case of **high correlated** dictionary.

To publish the paper: Ongoing!

To implement other OR stuffs in the current branch-and-bound framework;

To tackle other specific problems: e.g. structured sparsity, ...

Thank you for your attention

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