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On the properties of the solution path of the constrained and penalized L2-L0 problems

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1 Domain of optimization

For $k \leq n$, we define the domain $\mathcal{D}_k \subset \mathbb{R}^n$:

$$\mathcal{D}_k = \{\mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\|_0 = k\}. \quad (1)$$

Theorem 1 For $k \geq 1$, \mathcal{D}_k is not a closed set, and $\overline{\mathcal{D}_k} = \{\mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\|_0 \leq k\}$ (denoting by $\overline{\cdot}$ the closure operator).

Proof 1 • \mathcal{D}_k is not a closed set: it is easy to find a sequence $\mathbf{x}_j \in \mathcal{D}_k$ ($j \in \mathbb{N}$) whose limit is not in \mathcal{D}_k . For instance, $\mathbf{x}_j = (1/j)\mathbf{e}$, where \mathbf{e} is a given vector in \mathcal{D}_k . \mathbf{x}_j tends towards $\mathbf{0} \notin \mathcal{D}_k$.

- $\overline{\mathcal{D}_k} \subseteq \{\mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\|_0 \leq k\}$. If $\mathbf{x} \in \overline{\mathcal{D}_k}$, then there exists a sequence $\mathbf{x}_j \in \mathcal{D}_k$ ($j \in \mathbb{N}$) whose limit is equal to \mathbf{x} . Then,

$$\forall \varepsilon > 0, \exists J, j \geq J \Rightarrow \forall i, |\mathbf{x}(i) - \mathbf{x}_j(i)| < \varepsilon.$$

Applying this property with $\varepsilon = \min_{\mathbf{x}(i) \neq 0} |\mathbf{x}(i)|$, we deduce that there exists an iteration J , such that $\forall j \geq J, \forall i, \mathbf{x}(i) \neq 0 \Rightarrow \mathbf{x}_j(i) \neq 0$. In other words, $\|\mathbf{x}\|_0 \leq \|\mathbf{x}_j\|_0 = k$.

- $\{\mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\|_0 \leq k\} \subseteq \overline{\mathcal{D}_k}$. Let us show that if \mathbf{x} is such that $\|\mathbf{x}\|_0 \leq k$, then there exists a sequence $\mathbf{x}_j \in \mathcal{D}_k$ whose limit is equal to \mathbf{x} . Given \mathbf{x} , we define \mathbf{x}_j by setting $\mathbf{x}_j(i) = \mathbf{x}(i)$ if $i \in \mathcal{A}(\mathbf{x})$ (support of \mathbf{x}), and by replacing the $k - \|\mathbf{x}\|_0$ first zero valued entries of \mathbf{x} by $1/j$ in \mathbf{x}_j , and setting to 0 the remaining $n - k$ entries $\mathbf{x}_j(i)$. Obviously, $\mathbf{x}_j \in \mathcal{D}_k$ and this sequence tends towards \mathbf{x} .

The consequence of theorem 1 is that

$$\arg \min_{\mathbf{x} \in \mathcal{D}_k} \{\mathcal{E}(\mathbf{x}) = \|\mathbf{y} - \mathbf{A}\mathbf{x}\|^2\}$$

is not always defined, although the minimal value $\min_{\mathbf{x} \in \mathcal{D}_k} \mathcal{E}(\mathbf{x})$ is defined. On the contrary, the set of minimizers

$$\mathcal{X}_c(k) = \arg \min_{\mathbf{x} \in \overline{\mathcal{D}_k}} \mathcal{E}(\mathbf{x}) = \arg \min_{\|\mathbf{x}\|_0 \leq k} \mathcal{E}(\mathbf{x})$$

is properly defined because $\overline{\mathcal{D}_k}$ is a closed set and \mathcal{E} is quadratic and convex (to be completed).

Example 1 Let us consider the minimization of $\|\mathbf{x}\|^2$ over the domain \mathcal{D}_k . For $k \geq 1$, there is no minimizer over \mathcal{D}_k , but the minimal cost $\min_{\mathbf{x} \in \mathcal{D}_k} \|\mathbf{x}\|^2$ is equal to 0. The set of minimizers over $\overline{\mathcal{D}_k}$ is reduced to one vector: $\mathcal{X}_c(k) = \{\mathbf{0}\}$.

Example 2 The set $\mathcal{X}_c(k)$ is not always a singleton. Let us consider the minimization of the 2D cost function $\mathcal{E}(\mathbf{x}) = \mathbf{x}(1)^2$. It is easy to see that $\mathcal{X}_c(0) = \{\mathbf{0}\}$, $\mathcal{X}_c(1) = \{[0, \mathbf{x}(2)]^T, \mathbf{x}(2) \in \mathbb{R}\}$ and $\mathcal{X}_c(2) = \mathcal{X}_c(1)$.

Example 3 Let us consider the minimization of the 2D cost function $\mathcal{E}(\mathbf{x}) = (\mathbf{x}(1) - \alpha)^2$ for a given $\alpha \neq 0$. It is easy to see that $\mathcal{X}_c(0) = \{\mathbf{0}\}$, $\mathcal{X}_c(1) = \{[\alpha, 0]^T\}$ and $\mathcal{X}_c(2) = \{[\alpha, \mathbf{x}(2)]^T, \mathbf{x}(2) \in \mathbb{R}\}$.

Remark 1 Obviously, the sets $\overline{\mathcal{D}_k}$ have a nesting property ($\overline{\mathcal{D}_k} \subset \overline{\mathcal{D}_{k+1}}$), therefore, for all k , we have

$$\forall \mathbf{x}_k \in \mathcal{X}_c(k), \forall \mathbf{x}_{k+1} \in \mathcal{X}_c(k+1), \mathcal{E}(\mathbf{x}_{k+1}) \leq \mathcal{E}(\mathbf{x}_k).$$

Theorem 2 $\mathcal{X}_c(k+1) \cap \overline{\mathcal{D}_k} \subseteq \mathcal{X}_c(k)$.

Proof 2 Let us consider $\mathbf{x}_{k+1} \in \mathcal{X}_c(k+1) \cap \overline{\mathcal{D}_k}$. Since $\overline{\mathcal{D}_k} \subset \overline{\mathcal{D}_{k+1}}$ and \mathbf{x}_{k+1} is a minimizer of \mathcal{E} over $\overline{\mathcal{D}_{k+1}}$, we have $\forall \mathbf{x} \in \overline{\mathcal{D}_k}$, $\mathcal{E}(\mathbf{x}_{k+1}) \leq \mathcal{E}(\mathbf{x})$. As $\mathbf{x}_{k+1} \in \overline{\mathcal{D}_k}$, \mathbf{x}_{k+1} is a minimizer of \mathcal{E} over $\overline{\mathcal{D}_k}$.

2 Working assumptions and notion of constrained solution path

2.1 Unique representation property

We recall the definition of the unique representation property (URP), introduced in [1] in the underdetermined case (when $m \leq n$):

Definition 1 A matrix \mathbf{A} of size $m \times n$ ($m \leq n$) satisfies the URP if and only if any selection of m columns of \mathbf{A} forms a family of linearly independent vectors.

Under the URP assumption, we can solve $\mathbf{y} = \mathbf{A}\mathbf{x}$ by imposing that $\mathbf{x} \in \overline{\mathcal{D}_m}$. The system is then equivalent to $\mathbf{y} = \mathbf{B}\mathbf{z}$ where \mathbf{B} is a matrix of size $m \times m$ extracted from \mathbf{A} , and \mathbf{z} is the corresponding vector extracted from \mathbf{x} , of size $m \times 1$. According to the URP definition, \mathbf{B} is always invertible, and we can find sparse solutions to $\mathbf{y} = \mathbf{A}\mathbf{x}$ with at most m non-zero entries ($\mathbf{z} = \mathbf{B}^{-1}\mathbf{y}$ and then $\mathbf{x} = \{\mathbf{z}, \mathbf{0}\}$ for all the possible extractions \mathbf{B} from \mathbf{A}).

When $m > n$, we adopt the following definition:

Definition 2 A matrix \mathbf{A} of size $m \times n$ ($m > n$) satisfies the URP if and only if it is full rank.

When $m > n$, there is generally no solution to $\mathbf{y} = \mathbf{A}\mathbf{x}$ but the minimizer of $\mathcal{E}(\mathbf{x})$ over \mathbb{R}^n is unique (although not necessarily sparse): $\mathcal{X}_c(n) = \{(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{y}\}$.

In the following, we will assume that $\mathbf{y} \neq \mathbf{0}$ and that \mathbf{A} satisfies the URP.

2.2 Cardinality of the set $\mathcal{X}_c(k)$

Theorem 3 For $k \leq \min(m, n)$, the set $\mathcal{X}_c(k)$ is finite under the URP assumption.

Proof 3 Because of the URP assumption, any selection of $k \leq \min(m, n)$ columns of \mathbf{A} yields a matrix \mathbf{B} of size $m \times k$ whose rank is equal to k . Then, the energy reduces to $\mathcal{E}(\mathbf{x}) = \mathcal{E}(\mathbf{z}; \mathbf{0}) = \|\mathbf{y} - \mathbf{B}\mathbf{z}\|^2$ (where $\mathbf{z} \in \mathbb{R}^k$), and there is only one minimizer of $\mathbf{z} \mapsto \mathcal{E}(\mathbf{z}; \mathbf{0})$ over \mathbb{R}^k . Since the number of possible selections of k columns of \mathbf{A} is finite, the set $\mathcal{X}_c(k)$ is finite.

Remark 2 The minimal value of $\mathcal{E}(\mathbf{x})$ (for $\mathbf{x} \in \mathbb{R}^n$) can be reached when minimizing \mathcal{E} over $\overline{\mathcal{D}_{\min(m, n)}}$. Thus, when $m \leq n$, it is not necessary to compute $\mathcal{X}_c(k)$ for $k > m$. According to theorem 3, when $m > n$, all the sets $\mathcal{X}_c(k)$, $k = 0, \dots, n$ are finite.

Theorem 4 When $m \leq n$ and k is such that $m < k \leq n$, the set $\mathcal{X}_c(k)$ is of infinite cardinality.

Proof 4 Given a solution $\mathbf{x}_m \in \mathcal{X}_c(m)$, let $\mathcal{A}(\mathbf{x}_m)$ be the support of \mathbf{x}_m . We consider a support \mathcal{B} of cardinality k such that $\mathcal{A}(\mathbf{x}_m) \subset \mathcal{B} \subseteq \{1, \dots, n\}$, and we extract from \mathbf{A} the matrix \mathbf{B} of size $m \times k$ formed of the columns \mathbf{a}_i of \mathbf{A} ($i \in \mathcal{B}$). Then, let us add to \mathbf{x}_m a vector \mathbf{n} belonging to the null space of \mathbf{B} . Clearly, $\mathbf{x}_m + \mathbf{n} \in \mathcal{X}_c(k)$ because $\|\mathbf{x}_m + \mathbf{n}\|_0 \leq k$ and $\mathcal{E}(\mathbf{x}_m + \mathbf{n}) = \mathcal{E}(\mathbf{x}_m) = \min_{\mathbf{x} \in \mathbb{R}^n} \mathcal{E}(\mathbf{x})$. Since the null space of \mathbf{B} is of dimension $k - m > 0$, $\mathcal{X}_c(k)$ is of infinite cardinality.

As a conclusion, the constrained solution path is defined in the following way, for any case ($m \leq n$ or $m > n$).

Definition 3 *The constrained solution path is the (finite) set*

$$\mathcal{X}_c = \bigcup_{k=0}^{\min(m,n)} \mathcal{X}_c(k).$$

3 Properties of the penalized solution path

3.1 Penalized solution path

For a given $\lambda \geq 0$, we define the set of minimizers of $\mathcal{J}(\mathbf{x}; \lambda) = \mathcal{E}(\mathbf{x}) + \lambda \|\mathbf{x}\|_0$:

$$\mathcal{X}_p(\lambda) = \arg \min_{\mathbf{x} \in \mathbb{R}^n} \{\mathcal{J}(\mathbf{x}; \lambda)\}.$$

By extension, we define $\mathcal{X}_p(+\infty) = \{\mathbf{0}\}$.

Definition 4 *We denote the cardinality of a set $\mathcal{A} \subseteq \{1, \dots, n\}$ by*

$$\|\mathcal{A}\|_0 \triangleq \text{Card}(\mathcal{A}).$$

Definition 5 *We denote by $\mathcal{A}(\mathbf{x}) \subseteq \{1, \dots, n\}$ the support of a vector $\mathbf{x} \in \mathbb{R}^n$.*

Definition 6 *For a given active set \mathcal{A} such that $\|\mathcal{A}\|_0 \leq \min(m, n)$, the corresponding least-square solution is unique (due to the URP assumption). We denote this solution by*

$$\mathbf{x}_{\mathcal{A}} \triangleq \arg \min_{\mathcal{A}(\mathbf{x}) \subseteq \mathcal{A}} \mathcal{E}(\mathbf{x}) \quad (2)$$

and the corresponding least-square cost by

$$\mathcal{E}_{\mathcal{A}} \triangleq \mathcal{E}(\mathbf{x}_{\mathcal{A}}) = \min_{\mathcal{A}(\mathbf{x}) \subseteq \mathcal{A}} \mathcal{E}(\mathbf{x}). \quad (3)$$

Finally, we define the corresponding value of \mathcal{J} by

$$\mathcal{J}_{\mathcal{A}}(\lambda) \triangleq \mathcal{J}(\mathbf{x}_{\mathcal{A}}; \lambda) = \mathcal{E}_{\mathcal{A}} + \lambda \|\mathbf{x}_{\mathcal{A}}\|_0 \quad (4)$$

which is generally different from

$$\min_{\mathcal{A}(\mathbf{x}) \subseteq \mathcal{A}} \mathcal{J}(\mathbf{x}; \lambda).$$

Theorem 5 *If $\lambda > 0$ and $\mathbf{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$, then the support of $\mathbf{x}_p(\lambda)$, denoted by $\mathcal{A} \triangleq \mathcal{A}(\mathbf{x}_p(\lambda))$ for convenience, is such that $\|\mathcal{A}\|_0 \leq \min(m, n)$, and $\mathbf{x}_p(\lambda) = \mathbf{x}_{\mathcal{A}}$.*

Proof 5 — *First, we show that*

$$\mathbf{x}_p(\lambda) \in \arg \min_{\{\mathbf{x} \in \mathbb{R}^n, \mathcal{A}(\mathbf{x}) \subseteq \mathcal{A}\}} \mathcal{E}(\mathbf{x}).$$

Since $\mathbf{x}_p(\lambda)$ is a minimizer of $\mathcal{J}(\mathbf{x}; \lambda)$, the following equivalent inequalities hold for all \mathbf{x} such that $\mathcal{A}(\mathbf{x}) \subseteq \mathcal{A}$:

$$\begin{aligned} \mathcal{J}(\mathbf{x}; \lambda) &\geq \mathcal{J}(\mathbf{x}_p(\lambda); \lambda) \\ \mathcal{E}(\mathbf{x}) + \lambda \|\mathbf{x}\|_0 &\geq \mathcal{E}(\mathbf{x}_p(\lambda)) + \lambda \|\mathcal{A}\|_0 \\ \mathcal{E}(\mathbf{x}) - \mathcal{E}(\mathbf{x}_p(\lambda)) &\geq \lambda (\|\mathcal{A}\|_0 - \|\mathbf{x}\|_0) \geq 0. \end{aligned}$$

We finally deduce that $\mathbf{x}_p(\lambda)$ is a minimizer of \mathcal{E} over the set $\{\mathbf{x} \in \mathbb{R}^n, \mathcal{A}(\mathbf{x}) \subseteq \mathcal{A}\}$.

— *The case where $\|\mathcal{A}\|_0 > \min(m, n)$ never occurs. If it does, remark 2 shows that there exists $\mathbf{x} \in \overline{\mathcal{D}_{\min(m,n)}}$ such that $\mathcal{E}(\mathbf{x}) = \mathcal{E}(\mathbf{x}_p(\lambda))$. Since $\|\mathbf{x}\|_0 \leq \min(m, n) < \|\mathbf{x}_p(\lambda)\|_0 = \|\mathcal{A}\|_0$, $\mathcal{J}(\mathbf{x}; \lambda) < \mathcal{J}(\mathbf{x}_p(\lambda); \lambda)$, which is in contradiction with $\mathbf{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$.*

Finally, $\|\mathcal{A}\|_0 \leq \min(m, n)$ and there is only one minimizer of \mathcal{E} over the set $\{\mathbf{x} \in \mathbb{R}^n, \mathcal{A}(\mathbf{x}) \subseteq \mathcal{A}\}$ (URP assumption), which is $\mathbf{x}_{\mathcal{A}}$.

Corrolary 1 If $\lambda > 0$, the set $\mathcal{X}_p(\lambda)$ is finite and $\mathcal{X}_p(\lambda) \subseteq \overline{\mathcal{D}_{\min(m,n)}}$.

Proof 6 There are at most $\sum_{k=0}^{\min(m,n)} C_n^k$ distinct values $\mathbf{x}_p(\lambda)$ (i.e., $\sum_{k=0}^{\min(m,n)} C_n^k$ sets which are candidate to be a set \mathcal{A} and one optimal \mathbf{x} -value $\mathbf{x}_\mathcal{A}$ per set), which shows that $\mathcal{X}_p(\lambda)$ is a finite set. Additionally, we have seen in theorem 5 that for each solution $\mathbf{x}_p(\lambda)$, $\|\mathbf{x}_p(\lambda)\|_0 = \|\mathcal{A}\|_0 \leq \min(m, n)$.

Definition 7 The penalized solution path is defined as the union of sets

$$\mathcal{X}_p = \bigcup_{\lambda > 0} \mathcal{X}_p(\lambda).$$

Imposing $\lambda > 0$ (rather than $\lambda \geq 0$) guarantees that $\mathcal{X}_p(\lambda)$ is of finite cardinality for all λ . Moreover, it is easy to see (from theorem 5) that the solution path is of finite cardinality, since all the sets $\mathcal{X}_p(\lambda)$ are included in a common set of cardinality $\sum_{k=0}^{\min(m,n)} C_n^k$: $\{\mathbf{x} \in \mathbb{R}^n, \exists \mathcal{A} \subseteq \{1, \dots, n\}, \|\mathcal{A}\|_0 \leq \min(m, n) \text{ and } \mathbf{x} = \mathbf{x}_\mathcal{A}\}$.

3.2 Piecewise constant property

Theorem 6 The dependence of the set $\mathcal{X}_p(\lambda)$ w.r.t. λ ($\lambda > 0$) is piecewise constant, with a finite number of intervals $(\lambda_i^*, \lambda_{i+1}^*)$: for all i , $\mathcal{X}_p(\lambda)$ is constant for $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$ and if $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$, then $\mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(\lambda_i^*) \cap \mathcal{X}_p(\lambda_{i+1}^*)$.

The minimal cost value $\mathcal{J}(\lambda) \triangleq \min_{\mathbf{x} \in \mathbb{R}^n} \mathcal{J}(\mathbf{x}; \lambda)$ is a continuous and piecewise linear function of λ , and

$$\forall \lambda, \mathcal{J}(\lambda) = \min_{\{\mathcal{A} \subseteq \{1, \dots, n\}, \|\mathcal{A}\|_0 \leq \min(m, n)\}} \mathcal{J}_\mathcal{A}(\lambda). \quad (5)$$

Definition 8 In the following, we will define the values $\lambda = \lambda_i^*$ ($i = 1, \dots, I$) as the **critical values**. These values, together with $\lambda_0^* = 0$ and $\lambda_{I+1}^* = +\infty$, define the piecewise constant domain $\mathcal{X}_p(\lambda)$:

$$0 = \lambda_0^* < \lambda_1^* < \dots < \lambda_I^* < \lambda_{I+1}^* = +\infty. \quad (6)$$

λ_i^* are also the λ -values at which the derivative of \mathcal{J} is changing: at $\lambda = \lambda_i^*$, $\lambda \mapsto \mathcal{J}(\lambda)$ is not differentiable, and \mathcal{J} is linear on each interval $[\lambda_i^*, \lambda_{i+1}^*]$ (see Fig. 1).

Proof 7 — The result (5) can be illustrated geometrically, by considering the affine curves $\lambda \mapsto \mathcal{J}_\mathcal{A}(\lambda)$ for all the possible supports \mathcal{A} such that $\|\mathcal{A}\|_0 \leq \min(m, n)$ (see Fig. 1). Let us prove that (5) holds.

When λ is fixed, let $\mathbf{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$, and let $\mathcal{A} \triangleq \mathcal{A}(\mathbf{x}_p(\lambda))$.

- According to theorem 5, $\|\mathbf{x}_p(\lambda)\|_0 = \|\mathcal{A}\|_0 \leq \min(m, n)$ and $\mathbf{x}_p(\lambda) = \mathbf{x}_\mathcal{A}$. Thus, $\mathcal{E}(\mathbf{x}_p(\lambda)) = \mathcal{E}_\mathcal{A}$ and

$$\mathcal{J}(\mathbf{x}_p(\lambda); \lambda) = \mathcal{J}_\mathcal{A}(\lambda).$$

- $\mathbf{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$ implies that for all $\mathcal{A}' \subseteq \{1, \dots, n\}$ such that $\|\mathcal{A}'\|_0 \leq \min(m, n)$,

$$\mathcal{J}(\mathbf{x}_p(\lambda); \lambda) \leq \mathcal{J}_{\mathcal{A}'}(\lambda) = \mathcal{J}(\mathbf{x}_{\mathcal{A}'}; \lambda).$$

Here, we have shown that (5) holds since $\mathcal{J}(\lambda) = \mathcal{J}(\mathbf{x}_p(\lambda); \lambda)$.

— $\lambda \mapsto \mathcal{J}(\lambda)$ is a continuous and piecewise linear function of λ because of (5). Since the number of affine curves $\lambda \mapsto \mathcal{J}_\mathcal{A}(\lambda)$ is finite, $\lambda \mapsto \mathcal{J}(\lambda)$ is described by a finite set of values $\{(\lambda_i^*, \mathcal{E}_{\mathcal{A}_i}, \|\mathbf{x}_{\mathcal{A}_i}\|_0), i = 0, \dots, I\}$, where $\lambda_0^* = 0 < \lambda_1^* < \dots < \lambda_I^* < \lambda_{I+1}^* = +\infty$. Each value λ_i^* ($i = 1, \dots, I$) corresponds to the intersection between a pair of affine curves (see Fig. 1), and the restriction of \mathcal{J} to a given interval $[\lambda_i^*, \lambda_{i+1}^*]$ is linear:

$$\forall \lambda \in [\lambda_i^*, \lambda_{i+1}^*], \mathcal{J}(\lambda) = \mathcal{E}_{\mathcal{A}_i} + \lambda \|\mathbf{x}_{\mathcal{A}_i}\|_0. \quad (7)$$

In particular, for $i = 0$, we have

$$\forall \lambda \in [0, \lambda_1], \mathcal{J}(\lambda) = \mathcal{E}_{\mathcal{A}_0} + \lambda \|\mathbf{x}_{\mathcal{A}_0}\|_0, \quad (8)$$

where $\mathcal{E}_{\mathcal{A}_0} = \min_{\mathbf{x} \in \mathbb{R}^n} \mathcal{E}(\mathbf{x})$ is the minimal least-square error, and $\|\mathbf{x}_{\mathcal{A}_0}\|_0$ is the minimal L_0 -norm of the minimizers of \mathcal{E} over \mathbb{R}^n . For $i = I$, we have necessarily $\mathbf{x}_{\mathcal{A}_I} = \mathbf{0}$ and $\mathcal{E}_{\mathcal{A}_I} = \|\mathbf{y}\|^2$, thus

$$\forall \lambda \in [\lambda_I^*, +\infty), \mathcal{J}(\lambda) = \|\mathbf{y}\|^2. \quad (9)$$

— For a given interval $[\lambda_i^*, \lambda_{i+1}^*]$, let us show that when $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$, $\mathcal{X}_p(\lambda)$ is a constant set. For some given λ -value $\in (\lambda_i^*, \lambda_{i+1}^*)$, we consider $\mathbf{x} \in \mathcal{X}_p(\lambda)$, then necessarily, the following equivalent equations hold:

$$\begin{aligned} \mathcal{J}(\lambda) &= \mathcal{J}(\mathbf{x}; \lambda) \\ \mathcal{E}_{\mathcal{A}_i} + \lambda \|\mathbf{x}_{\mathcal{A}_i}\|_0 &= \mathcal{E}(\mathbf{x}) + \lambda \|\mathbf{x}\|_0. \end{aligned}$$

Imagine that $\mathcal{E}_{\mathcal{A}_i} \neq \mathcal{E}(\mathbf{x})$, then, necessarily, the two functions $\mathcal{J}(\lambda') = \mathcal{E}_{\mathcal{A}_i} + \lambda' \|\mathbf{x}_{\mathcal{A}_i}\|_0$ and $\mathcal{J}(\mathbf{x}; \lambda') = \mathcal{E}(\mathbf{x}) + \lambda' \|\mathbf{x}\|_0$ do not coincide for $\lambda' \in [\lambda_i^*, \lambda_{i+1}^*] \setminus \{\lambda\}$. Moreover, $\mathcal{J}(\mathbf{x}; \lambda')$ is strictly lower than $\mathcal{J}(\lambda')$ either for $\lambda' \in [\lambda_i^*, \lambda)$ or for $\lambda' \in (\lambda, \lambda_{i+1}^*]$. This is in contradiction with (7) and the definition of $\mathcal{J}(\lambda')$ in theorem 6.

We have shown that $\mathcal{E}_{\mathcal{A}_i} = \mathcal{E}(\mathbf{x})$. Since $\mathcal{J}(\lambda) = \mathcal{J}(\mathbf{x}; \lambda)$ and $\lambda > 0$, we deduce that $\|\mathbf{x}_{\mathcal{A}_i}\|_0 = \|\mathbf{x}\|_0$, and that $\forall \lambda' \in [\lambda_i^*, \lambda_{i+1}^*]$, $\mathcal{J}(\lambda') = \mathcal{J}(\mathbf{x}; \lambda')$. Finally, if $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$ and $\mathbf{x} \in \mathcal{X}_p(\lambda)$, then $\mathbf{x} \in \mathcal{X}_p(\lambda')$ for all $\lambda' \in [\lambda_i^*, \lambda_{i+1}^*]$. $\mathcal{X}_p(\lambda)$ is then a constant set when $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$, and $\mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(\lambda_i^*) \cap \mathcal{X}_p(\lambda_{i+1}^*)$.

Lemma 1 The function $\lambda \mapsto \mathcal{J}(\lambda)$ is increasing and concave.

Proof 8 \mathcal{J} is an increasing and concave function as the minimum of a finite set of increasing and concave functions.

Lemma 2 $\mathcal{X}_p(0) \cap \mathcal{X}_p \neq \emptyset$, and if $m \geq n$, then $\mathcal{X}_p(0) \subset \mathcal{X}_p$.

Proof 9 The application of the result of theorem 6: “for all i , if $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$, then $\mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(\lambda_i^*)$ ” with $i = 0$ yields

$$\forall \lambda \in (0, \lambda_1^*), \mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(0).$$

Thus, we always have $\mathcal{X}_p(0) \cap \mathcal{X}_p \neq \emptyset$. For $m \geq n$, $\mathcal{X}_p(0)$ is formed of only one vector, thus $\forall \lambda \in (0, \lambda_1^*)$, $\mathcal{X}_p(\lambda) = \mathcal{X}_p(0)$, and $\mathcal{X}_p(0) \subseteq \mathcal{X}_p$. Since $\mathbf{y} \neq \mathbf{0}$ and \mathbf{A} is full rank, the domain (6) is formed of at least two intervals ($I \geq 1$), thus $\mathcal{X}_p(0) \subset \mathcal{X}_p$.

Theorem 7 For a given λ -value which is distinct from $\lambda_0^*, \lambda_1^*, \dots, \lambda_I^*$, all the elements of $\mathcal{X}_p(\lambda)$ are of same L_0 -norm, which is equal to the derivative of $\mathcal{J}(\lambda)$, and yield the same least-square cost.

Proof 10 Because of theorem 6, for a given value of i , there exists $\mathcal{A}_i \subseteq \{1, \dots, n\}$ such that

$$\forall \lambda' \in [\lambda_i^*, \lambda_{i+1}^*], \mathcal{J}(\lambda') = \mathcal{J}_{\mathcal{A}_i}(\lambda'). \quad (10)$$

Now, let us fix the value of $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$ and let $\mathbf{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$. Because of theorem 6, $\mathcal{X}_p(\lambda')$ is constant for $\lambda' \in (\lambda_i^*, \lambda_{i+1}^*)$, and $\mathbf{x}_p(\lambda) \in \mathcal{X}_p(\lambda')$ for all $\lambda' \in [\lambda_i^*, \lambda_{i+1}^*]$. (10) implies that

$$\begin{aligned} \forall \lambda' \in [\lambda_i^*, \lambda_{i+1}^*], \mathcal{J}(\mathbf{x}_p(\lambda); \lambda') &= \mathcal{J}_{\mathcal{A}_i}(\lambda') \\ \forall \lambda' \in [\lambda_i^*, \lambda_{i+1}^*], \mathcal{E}(\mathbf{x}_p(\lambda)) + \lambda' \|\mathbf{x}_p(\lambda)\|_0 &= \mathcal{E}_{\mathcal{A}_i} + \lambda' \|\mathbf{x}_{\mathcal{A}_i}\|_0. \end{aligned} \quad (11)$$

Taking the derivative of (11) yields $\|\mathbf{x}_p(\lambda)\|_0 = \|\mathbf{x}_{\mathcal{A}_i}\|_0 = \mathcal{J}'(\lambda)$, and then, due to (11), $\mathcal{E}(\mathbf{x}_p(\lambda)) = \mathcal{E}_{\mathcal{A}_i}$.

Theorem 8 Let $\mathbf{x}_p(\lambda)$ be a sequence such that $\forall \lambda, \mathbf{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$. Then, necessarily, $\|\mathbf{x}_p(\lambda)\|_0$ is a decreasing function of λ , and $\mathcal{E}(\mathbf{x}_p(\lambda))$ is an increasing function of λ .

Proof 11 • Recall that for $i \in \{0, \dots, I\}$, there exists a set \mathcal{A}_i such that if $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$ and $\mathbf{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$, then $\|\mathbf{x}_p(\lambda)\|_0 = \|\mathbf{x}_{\mathcal{A}_i}\|_0$ (see theorem 7);

- The first result is a direct consequence of theorem 7: $\forall \lambda \notin \{\lambda_0^*, \dots, \lambda_I^*\}$, $\|\mathbf{x}_p(\lambda)\|_0 = \mathcal{J}'(\lambda)$, and of lemma 1: \mathcal{J} is a concave function, thus its derivative (when it is defined) is a decreasing function of λ . At this point, we know that $\lambda \mapsto \|\mathbf{x}_p(\lambda)\|_0$ is piecewise constant on \mathbb{R}_+ , and that its restriction to $\mathbb{R}_+ \setminus \{\lambda_0^*, \dots, \lambda_I^*\}$ is decreasing: $\forall i \in \{1, \dots, I\}$, $\|\mathbf{x}_{\mathcal{A}_{i-1}}\|_0 \geq \|\mathbf{x}_{\mathcal{A}_i}\|_0$. The remaining part is to study the behavior of $\|\mathbf{x}_p(\lambda)\|_0$ at $\lambda = \lambda_i^*$, $i = 0, \dots, I$.

For $i \in \{1, \dots, I\}$, let us show that $\mathbf{x}_p(\lambda_i^*)$ is such that $\|\mathbf{x}_{\mathcal{A}_{i-1}}\|_0 \geq \|\mathbf{x}_p(\lambda_i^*)\|_0 \geq \|\mathbf{x}_{\mathcal{A}_i}\|_0$:

- $\lambda \mapsto \mathcal{J}(\mathbf{x}_p(\lambda_i^*); \lambda)$ and $\lambda \mapsto \mathcal{J}(\lambda)$ coincide at $\lambda = \lambda_i^*$;
- $\mathcal{J}'(\lambda)$ is equal to $\|\mathbf{x}_{\mathcal{A}_{i-1}}\|_0$ when $\lambda \in (\lambda_{i-1}^*, \lambda_i^*)$, and to $\|\mathbf{x}_{\mathcal{A}_i}\|_0$ when $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$.
- the derivative of $\lambda \mapsto \mathcal{J}(\mathbf{x}_p(\lambda_i^*); \lambda)$ is equal to $\|\mathbf{x}_p(\lambda_i^*)\|_0$.

Due to the definition of $\lambda \mapsto \mathcal{J}(\lambda)$ in theorem 6, the affine function $\lambda \mapsto \mathcal{J}(\mathbf{x}_p(\lambda_i^*); \lambda)$ is necessarily greater or equal to $\lambda \mapsto \mathcal{J}(\lambda)$ for $\lambda \in (\lambda_{i-1}^*, \lambda_i^*)$ and for $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$. This implies that $\|\mathbf{x}_{\mathcal{A}_{i-1}}\|_0 \geq \|\mathbf{x}_p(\lambda_i^*)\|_0 \geq \|\mathbf{x}_{\mathcal{A}_i}\|_0$.

A similar argument can be given to show that $\|\mathbf{x}_p(\lambda_0^*)\|_0 \geq \|\mathbf{x}_{\mathcal{A}_0}\|_0$.

Finally, we have shown that $\lambda \mapsto \|\mathbf{x}_p(\lambda)\|_0$ is decreasing on \mathbb{R}_+ .

- Second result: for a given $i \in \{1, \dots, I\}$, the continuity of \mathcal{J} at $\lambda = \lambda_i^*$ reads $\mathcal{E}_{\mathcal{A}_{i-1}} + \lambda_i^* \|\mathbf{x}_{\mathcal{A}_{i-1}}\|_0 = \mathcal{E}_{\mathcal{A}_i} + \lambda_i^* \|\mathbf{x}_{\mathcal{A}_i}\|_0$. Because $\|\mathbf{x}_{\mathcal{A}_{i-1}}\|_0 \geq \|\mathbf{x}_{\mathcal{A}_i}\|_0$, $\mathcal{E}_{\mathcal{A}_{i-1}} \leq \mathcal{E}_{\mathcal{A}_i}$.

When λ varies from 0 to $+\infty$ and $\lambda \notin \{\lambda_1^*, \dots, \lambda_I^*\}$, $\mathcal{E}(\mathbf{x}_p(\lambda))$ takes sequentially the values $\mathcal{E}_{\mathcal{A}_i}$, $i = 0, \dots, I$. Thus, the restriction of $\lambda \mapsto \mathcal{E}(\mathbf{x}_p(\lambda))$ to $\mathbb{R}_+ \setminus \{\lambda_1^*, \dots, \lambda_I^*\}$ is increasing. With similar arguments than in the first result, we can show that for $i \in \{1, \dots, I\}$, $\mathcal{E}_{\mathcal{A}_{i-1}} \leq \mathcal{E}(\mathbf{x}_p(\lambda_i^*)) \leq \mathcal{E}_{\mathcal{A}_i}$. Finally, $\lambda \mapsto \mathcal{E}(\mathbf{x}_p(\lambda))$ is increasing on \mathbb{R}_+ .

3.3 Cardinality of $\mathcal{X}_p(\lambda)$

It is easy to see that:

- For all $i \in \{1, \dots, I\}$, the cardinality of $\mathcal{X}_p(\lambda_i^*)$ is larger than 2, because at $\lambda = \lambda_i^*$, at least two distinct affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda) = \mathcal{E}_{\mathcal{A}} + \lambda \|\mathbf{x}_{\mathcal{A}}\|_0$ intersect (see Fig. 2).
- $\mathcal{X}_p(\lambda)$ is reduced to the unique vector $\mathbf{0}$ for the largest λ -values ($\lambda > \lambda_I^* \Rightarrow \mathcal{X}_p(\lambda) = \{\mathbf{0}\}$).
- For $\lambda = 0$ (the least-square error $\mathcal{E}(\mathbf{x})$ is minimized with no penalty), $\mathcal{X}_p(0)$ is either reduced to the unique vector $(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{y}$ when $m \geq n$, or is of infinite cardinality otherwise.

We conclude that at least for $m \geq n$, the cardinality of $\mathcal{X}_p(\lambda)$ is not monotonic w.r.t. λ .

3.4 Relationship between the constrained and the penalized solution paths

Generally, the solution paths \mathcal{X}_c and \mathcal{X}_p do not coincide. This is a consequence of the non-convexity of the L0-norm [2]. However, $\mathcal{X}_p \subseteq \mathcal{X}_c$ is always true (a well-known result in the literature of multi-objective optimization?).

In general, the proposition “ $\forall k, \exists \lambda, \mathcal{X}_c(k) \subseteq \mathcal{X}_p(\lambda)$ ” is false (see Fig. 1).

Theorem 9 *If $\lambda \neq \{\lambda_0^*, \dots, \lambda_I^*\}$, then there exists k such that $\mathcal{X}_p(\lambda) = \mathcal{X}_c(k)$.*

Proof 12 *For a given λ -value, let $\mathbf{x} \in \mathcal{X}_p(\lambda)$, let $\mathcal{A} \triangleq \mathcal{A}(\mathbf{x})$ denote the support of \mathbf{x} and $k_{\mathbf{x}} \triangleq \|\mathbf{x}\|_0 = \|\mathcal{A}\|_0$. According to theorem 5, $\|\mathcal{A}\|_0 \leq \min(m, n)$ and $\mathbf{x} = \mathbf{x}_{\mathcal{A}}$.*

– *Let us show that $\mathbf{x} \in \mathcal{X}_c(k_{\mathbf{x}})$. If $\mathbf{x} \notin \mathcal{X}_c(k_{\mathbf{x}})$, there exists a (minimal) support \mathcal{B} such that $\|\mathcal{B}\|_0 \leq k_{\mathbf{x}}$ and $\mathcal{E}_{\mathcal{B}} < \mathcal{E}(\mathbf{x}) = \mathcal{E}_{\mathcal{A}}$, then $\mathcal{J}(\mathbf{x}_{\mathcal{B}}; \lambda) < \mathcal{J}(\mathbf{x}_{\mathcal{A}}; \lambda)$. This is in contradiction with $\mathbf{x} \in \mathcal{X}_p(\lambda)$.*

At this point, we have shown that

$$\forall \lambda, \forall \mathbf{x} \in \mathcal{X}_p(\lambda), \exists k_{\mathbf{x}}, \mathbf{x} \in \mathcal{X}_c(k_{\mathbf{x}}),$$

or equivalently,

$$\mathcal{X}_p \subseteq \mathcal{X}_c.$$

– *The following of the proof requires the assumption $\lambda \neq \{\lambda_0^*, \dots, \lambda_I^*\}$. We have seen that if \mathbf{x} and $\mathbf{y} \in \mathcal{X}_p(\lambda)$, then $\mathbf{x} \in \mathcal{X}_c(k_{\mathbf{x}})$ and $\mathbf{y} \in \mathcal{X}_c(k_{\mathbf{y}})$. According to theorem 7, all the elements of $\mathcal{X}_p(\lambda)$ are of same L0-norm. Therefore, $k_{\mathbf{y}} = k_{\mathbf{x}}$. At this point, we have shown that*

$$\forall \lambda \neq \{\lambda_0^*, \dots, \lambda_I^*\}, \exists k_{\lambda}, \mathcal{X}_p(\lambda) \subseteq \mathcal{X}_c(k_{\lambda}).$$

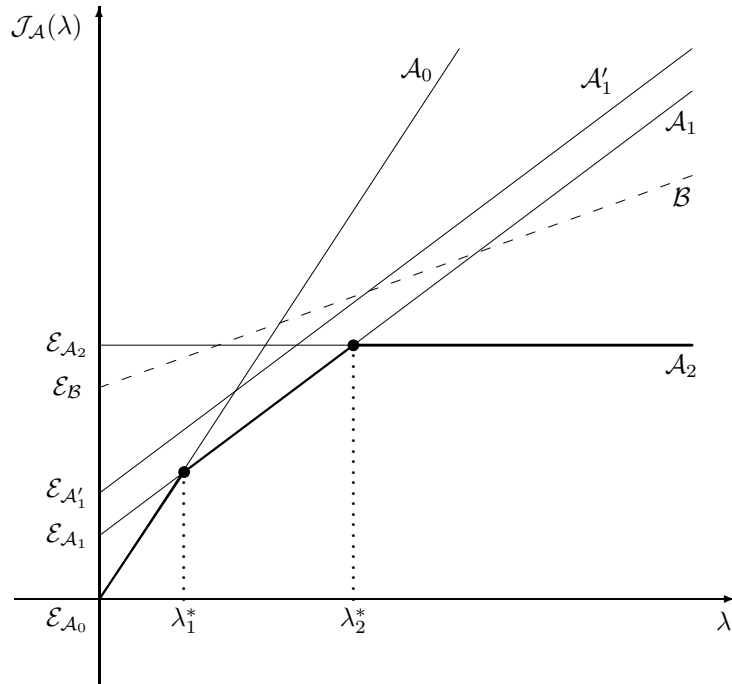


Figure 1: Representation of the affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda) = \mathcal{E}_{\mathcal{A}} + \lambda \|\mathbf{x}_{\mathcal{A}}\|_0$ for all the possible supports \mathcal{A} such that $\|\mathcal{A}\|_0 \leq \min(m, n)$. Note that a given affine curve may correspond to several supports \mathcal{A} and \mathcal{B} for which $\forall \lambda, \mathcal{J}_{\mathcal{A}}(\lambda) = \mathcal{J}_{\mathcal{B}}(\lambda)$. The piecewise linear function $\lambda \mapsto \mathcal{J}(\lambda)$ is defined according to (5) and is represented in bold lines. From this illustration, let us comment on the nonequivalence of both solution paths \mathcal{X}_c and \mathcal{X}_p . By following the bold curve representing $\lambda \mapsto \mathcal{J}(\lambda)$, we see that the penalized solution path is described by the active sets \mathcal{A}_0 , \mathcal{A}_1 and \mathcal{A}_2 (and the possible other sets yielding the same three curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}_i}(\lambda)$) for which $\|\mathbf{x}_{\mathcal{A}}\|_0$ is equal to 3, 2 and 0, respectively. \mathcal{A}'_1 is an active set such that $\|\mathbf{x}_{\mathcal{A}'_1}\|_0 = 2$ but $\mathcal{E}_{\mathcal{A}'_1} > \mathcal{E}_{\mathcal{A}_1}$. No active set such that $\|\mathbf{x}_{\mathcal{A}}\|_0 = 1$ is present in \mathcal{X}_p . \mathcal{B} is the active set such that $\|\mathbf{x}_{\mathcal{B}}\|_0 = 1$ whose energy $\mathcal{E}_{\mathcal{B}}$ is the lowest among all the active sets such that $\|\mathbf{x}_{\mathcal{A}}\|_0 \leq 1$, however, $\forall \lambda, \mathcal{J}_{\mathcal{B}}(\lambda) > \mathcal{J}(\lambda)$. Thus, $\mathcal{X}_c(1) = \{\mathcal{B}\} \not\subset \mathcal{X}_p$. On the contrary, for all $\lambda \neq \{\lambda_0^*, \dots, \lambda_l^*\}$, $\mathcal{X}_p(\lambda) = \mathcal{X}_c(k_\lambda)$, with $k_\lambda = \mathcal{J}'(\lambda) = 3, 2$ or 0 .

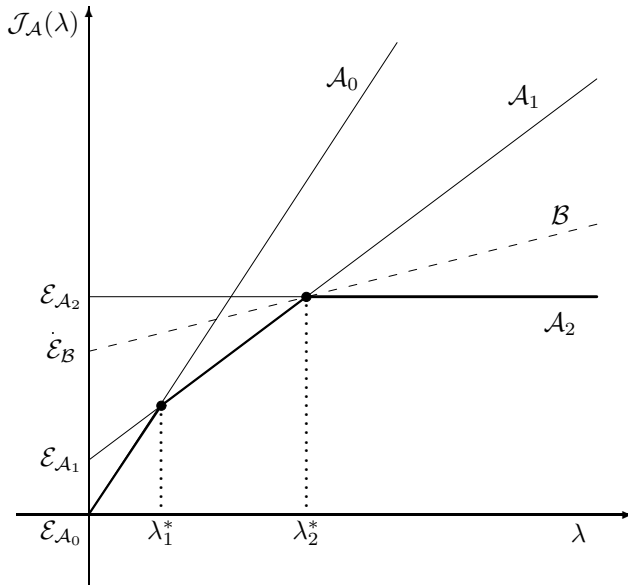


Figure 2: Content of $\mathcal{X}_p(\lambda)$ at a critical λ -value $\lambda = \lambda_i^*$, $i \geq 1$: $\mathcal{X}_p(\lambda_i^*) \subset \mathcal{X}_c$, and $\text{Card}(\mathcal{X}_p(\lambda_i^*)) \geq 2$. On this example, $\mathcal{X}_p(\lambda_2^*) = \mathcal{X}_c(0) \cup \mathcal{X}_c(1) \cup \mathcal{X}_c(2)$ and $\text{Card}(\mathcal{X}_p(\lambda_2^*)) \geq 3$ since \mathbf{x}_{A_1} , \mathbf{x}_{A_2} and $\mathbf{x}_B \in \mathcal{X}_p(\lambda_2^*)$.

— Now, let us prove the reverse inclusion. Given λ , there exists at least one \mathbf{x} such that $\mathbf{x} \in \mathcal{X}_p(\lambda)$, $k_\lambda = \|\mathbf{x}\|_0$ and $\mathbf{x} \in \mathcal{X}_c(k_\lambda)$. For all $\mathbf{y} \in \mathcal{X}_c(k_\lambda)$, we have necessarily $\mathcal{E}(\mathbf{y}) = \mathcal{E}(\mathbf{x})$ and $\|\mathbf{y}\|_0 \leq \|\mathbf{x}\|_0$, thus $\mathcal{J}(\mathbf{y}; \lambda) \leq \mathcal{J}(\mathbf{x}; \lambda)$. Since $\mathbf{x} \in \mathcal{X}_p(\lambda)$, we deduce that $\mathcal{J}(\mathbf{y}; \lambda) = \mathcal{J}(\mathbf{x}; \lambda)$ and that $\mathbf{y} \in \mathcal{X}_p(\lambda)$. This completes the proof, since we have shown that

$$\forall \lambda \neq \{\lambda_0^*, \dots, \lambda_I^*\}, \mathcal{X}_c(k_\lambda) \subseteq \mathcal{X}_p(\lambda).$$

Actually, $k_\lambda = \mathcal{J}'(\lambda)$ according to theorem 7.

3.5 Content of $\mathcal{X}_p(\lambda)$ at critical λ -values

Lemma 3 If $\lambda_{i-1}^* < \lambda < \lambda_i^* < \lambda' < \lambda_{i+1}^*$, then $\mathcal{X}_p(\lambda) \cap \mathcal{X}_p(\lambda') = \emptyset$.

Proof 13 According to theorem 7, all the vectors of $\mathcal{X}_p(\lambda)$ (respectively of $\mathcal{X}_p(\lambda')$) are of same L_0 -norm, which is the derivative of \mathcal{J} at λ (resp. λ'). Thus, if $\mathcal{X}_p(\lambda) \cap \mathcal{X}_p(\lambda') \neq \emptyset$, the derivative of \mathcal{J} is constant on $(\lambda_{i-1}^*, \lambda_{i+1}^*) \setminus \{\lambda_i^*\}$, which is in contradiction with the definition of λ_i^* (critical point, at which the derivative of \mathcal{J} is changing).

Theorem 10 If $\lambda_{i-1}^* < \lambda < \lambda_i^* < \lambda' < \lambda_{i+1}^*$, then $\mathcal{X}_p(\lambda) \cup \mathcal{X}_p(\lambda') \subseteq \mathcal{X}_p(\lambda_i^*)$, thus $\text{Card}(\mathcal{X}_p(\lambda)) + \text{Card}(\mathcal{X}_p(\lambda')) \leq \text{Card}(\mathcal{X}_p(\lambda_i^*))$ (Card denotes the cardinality). If $\lambda \in (\lambda_{i-1}^*, \lambda_{i+1}^*) \setminus \{\lambda_i^*\}$, then $\text{Card}(\mathcal{X}_p(\lambda)) < \text{Card}(\mathcal{X}_p(\lambda_i^*))$.

See illustration in Fig. 2.

Proof 14 • *First result:* according to theorem 6, if $\lambda \in (\lambda_i^*, \lambda_{i+1}^*)$, then $\mathcal{X}_p(\lambda) \subseteq \mathcal{X}_p(\lambda_i^*) \cap \mathcal{X}_p(\lambda_{i+1}^*)$. According to lemma 3, if $\lambda_{i-1}^* < \lambda < \lambda_i^* < \lambda' < \lambda_{i+1}^*$, then $\mathcal{X}_p(\lambda) \cap \mathcal{X}_p(\lambda') = \emptyset$. Thus, $\mathcal{X}_p(\lambda) \cup \mathcal{X}_p(\lambda') \subseteq \mathcal{X}_p(\lambda_i^*)$ and $\text{Card}(\mathcal{X}_p(\lambda)) + \text{Card}(\mathcal{X}_p(\lambda')) \leq \text{Card}(\mathcal{X}_p(\lambda_i^*))$.

- *Second result:* since neither $\mathcal{X}_p(\lambda)$ nor $\mathcal{X}_p(\lambda')$ is empty, their cardinality is larger or equal to 1, then, applying $\text{Card}(\mathcal{X}_p(\lambda)) + \text{Card}(\mathcal{X}_p(\lambda')) \leq \text{Card}(\mathcal{X}_p(\lambda_i^*))$, we deduce that $\text{Card}(\mathcal{X}_p(\lambda)) < \text{Card}(\mathcal{X}_p(\lambda_i^*))$ and $\text{Card}(\mathcal{X}_p(\lambda')) < \text{Card}(\mathcal{X}_p(\lambda_i^*))$.

4 SBR and CSBR algorithms

4.1 SBR iterates and output

Let us consider the SBR algorithm for a given λ -value. An SBR iterate takes the form of:

- an active set \mathcal{A} (for simplicity, we omit the dependence w.r.t. λ);
- the corresponding least-square minimizer $\mathbf{x}_{\mathcal{A}} = \arg \min_{\{\mathbf{x} \in \mathbb{R}^n, \mathcal{A}(\mathbf{x}) \subseteq \mathcal{A}\}} \mathcal{E}(\mathbf{x})$.

$\hat{\mathbf{x}}(\lambda) \triangleq \mathbf{x}_{\mathcal{A}}$ is chosen as the estimator of a minimizer (there may be several) of $\mathcal{J}(\mathbf{x}; \lambda) = \mathcal{E}(\mathbf{x}) + \lambda \|\mathbf{x}\|_0$ over \mathbb{R}^n .

First, recall that for the SBR iterates (and in particular when SBR terminates), $\|\mathbf{x}_{\mathcal{A}}\|_0 = \|\mathcal{A}\|_0$. This property can be guaranteed by including in the SBR loops a small procedure which removes from the active set \mathcal{A} all the indices $i \in \mathcal{A}$ such that $\mathbf{x}_{\mathcal{A}}(i) = 0$ (however, these removals rarely occur in practice). The following remark follows from this property.

Remark 3 For a given λ -value, the cost of an SBR iterate $\mathbf{x}_{\mathcal{A}}$ is $\mathcal{J}_{\mathcal{A}}(\lambda) = \mathcal{E}_{\mathcal{A}} + \lambda \|\mathcal{A}\|_0$. Because the cost of SBR iterates only depend on their support and for convenience, we will omit their dependence w.r.t. \mathbf{x} .

Remark 4 SBR terminates after a finite number of iterations. Moreover, a set \mathcal{A} cannot be explored twice while running SBR.

Proof 15 SBR is a descent algorithm and the number of sets \mathcal{A} which are reachable is finite (i.e., the number of subsets of $\{1, \dots, n\}$).

Remark 5 When SBR terminates, the estimate $\hat{\mathbf{x}}(\lambda) = \mathbf{x}_{\mathcal{A}}$ is generally not included in $\mathcal{X}_p(\lambda)$ because SBR is a sub-optimal algorithm.

Remark 6 At the SBR output \mathcal{A} , \mathcal{J} is “locally minimum w.r.t. \mathcal{A} ”: any replacement of \mathcal{A} by $\mathcal{A} \bullet i$ (where $\bullet \triangleq \cup$ or \setminus) does not yield a decrease of the cost $\mathcal{J}_{\mathcal{A}}(\lambda)$). Formally, this property reads:

$$\forall i, \mathcal{J}_{\mathcal{A}}(\lambda) \leq \mathcal{J}_{\mathcal{A} \bullet i}(\lambda), \quad (12)$$

or equivalently,

$$\begin{aligned} \forall i, \mathcal{E}_{\mathcal{A}} + \lambda \|\mathcal{A}\|_0 &\leq \mathcal{E}_{\mathcal{A} \bullet i} + \lambda \|\mathbf{x}_{\mathcal{A} \bullet i}\|_0 \\ \forall i, \mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \bullet i} &\leq \lambda (\|\mathbf{x}_{\mathcal{A} \bullet i}\|_0 - \|\mathcal{A}\|_0). \end{aligned} \quad (13)$$

Here, we do not consider the small removal procedure described above for $\mathcal{A} \bullet i$ (update of $\mathcal{A} \bullet i$ by removing the indices corresponding to the zero valued entries of $\mathbf{x}_{\mathcal{A} \bullet i}$), therefore we use $\|\mathbf{x}_{\mathcal{A} \bullet i}\|_0$, which may be lower than $\|\mathcal{A} \bullet i\|_0$.

4.2 Iterative computation of λ in the CSBR algorithm

When $\lambda = \lambda_q > 0$ (q -th call to SBR), let $\mathcal{A} = \mathcal{A}_q$ be the support of the output of SBR(λ_q). Then, (13) holds. For simplicity, we will omit, when possible, the dependence of \mathcal{A} w.r.t. q . When λ_q is replaced by another value $\lambda \leq \lambda_q$ and $\mathcal{A} = \mathcal{A}_q$ is kept fixed, for which λ -values does (13) remain valid?

When $\bullet = \setminus$, both terms on the left- and right-hand sides of the inequality are strictly negative ($\|\mathbf{x}_{\mathcal{A} \setminus i}\|_0 \leq \|\mathcal{A}\|_0 - 1$), while when $\bullet = \cup$, both terms are positive since $\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \cup i} \geq 0$ and (13) holds for $\lambda = \lambda_q$ (this implies that $\|\mathbf{x}_{\mathcal{A} \cup i}\|_0 = \|\mathcal{A}\|_0$ or $\|\mathcal{A}\|_0 + 1$). Therefore, (13) remains valid for $\lambda \neq \lambda_q$ if and only if

$$(0 \leq) \max_{i \notin \mathcal{A} \text{ and } \|\mathbf{x}_{\mathcal{A} \cup i}\|_0 = \|\mathcal{A}\|_0 + 1} (\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \cup i}) \leq \lambda \leq \min_{i \in \mathcal{A}} \left[\frac{\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \setminus i}}{\|\mathbf{x}_{\mathcal{A} \setminus i}\|_0 - \|\mathcal{A}\|_0} \right]. \quad (14)$$

The lower bound of (14) can be simplified to $\max_{i \notin \mathcal{A}} (\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \cup i})$ because if $i \notin \mathcal{A}$ is such that $\|\mathbf{x}_{\mathcal{A} \cup i}\|_0 = \|\mathcal{A}\|_0$, then (13) implies that $\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \cup i} = 0$. Thus, including these indices i in the computation of the lower bound of (14) does not change its value, and (14) simplifies to

$$\max_{i \notin \mathcal{A}} (\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \cup i}) \leq \lambda \leq \min_{i \in \mathcal{A}} \left[\frac{\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \setminus i}}{\|\mathbf{x}_{\mathcal{A} \setminus i}\|_0 - \|\mathcal{A}\|_0} \right]. \quad (15)$$

Given λ_q , the next λ -value $\lambda_{q+1} < \lambda_q$ is found by computing the lower bound of (15).

How to choose λ_{q+1} ? Setting λ_{q+1} to the lower bound of (15) is not judicious, since for this λ -value, \mathcal{J} is still “locally minimum w.r.t. \mathcal{A} ” in the sense of (12). One possibility is to set λ_{q+1} to the lower bound of (15) minus some $\varepsilon > 0$, without guarantee that this value is larger than the “next lower bound” of (15). Another possibility is to sort the values of

$$\tilde{\lambda}_i \triangleq \mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \cup i} \geq 0 \quad (16)$$

for all indices $i \notin \mathcal{A}$, and then to **set λ_{q+1} to the mean of the two largest values**. This setting ensures that the inequality $\tilde{\lambda}_i \leq \lambda_{q+1}$ does not hold for one value of $\tilde{\lambda}_i$ only.

- If the number of indices $i \notin \mathcal{A}$ such that $\tilde{\lambda}_i > 0$ is equal to 1, then we set λ_{q+1} to half of the value of $\tilde{\lambda}_i$.
- If all indices $i \notin \mathcal{A}$ are such that $\tilde{\lambda}_i = 0$, then we terminate CSBR.
- If \mathcal{A} is the complete set $\{1, \dots, n\}$, the lower bound of (15) is undefined, and we terminate CSBR.

Remark 7 For a given $i \notin \mathcal{A}$ for which $\|\mathbf{x}_{\mathcal{A} \cup i}\|_0 = \|\mathcal{A}\|_0 + 1$, $\tilde{\lambda}_i$ is the λ -value for which both affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{A} \cup i}(\lambda)$ intersect. Similarly, for $i \in \mathcal{A}$, the value

$$\tilde{\lambda}_i \triangleq \frac{\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \setminus i}}{\|\mathbf{x}_{\mathcal{A} \setminus i}\|_0 - \|\mathcal{A}\|_0} \quad (17)$$

is the λ -value for which both affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{A} \setminus i}(\lambda)$ intersect.

Proof 16 For $i \notin \mathcal{A}$ and for the λ -value $\tilde{\lambda}_i$, (13) is an equality, then $\mathcal{J}_{\mathcal{A}}(\tilde{\lambda}_i) = \mathcal{J}_{\mathcal{A} \cup i}(\tilde{\lambda}_i)$. Since $\|\mathbf{x}_{\mathcal{A} \cup i}\|_0$ is supposed to be different from $\|\mathcal{A}\|_0$, both affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{A} \cup i}(\lambda)$ are not parallel (their slopes are equal to $\|\mathcal{A}\|_0$ and $\|\mathbf{x}_{\mathcal{A} \cup i}\|_0 = \|\mathcal{A}\|_0 + 1$ respectively), and they intersect at $\lambda = \tilde{\lambda}_i$. A similar proof holds in the case where $i \in \mathcal{A}$ and \cup is replaced by \setminus .

Remark 8 A set \mathcal{A} of cardinality larger than $\min(m, n)$ cannot be explored.

Proof 17 — SBR: if a set \mathcal{A} of cardinality larger than $\min(m, n)$ is explored, then SBR has earlier explored at least one set \mathcal{B} of cardinality $\min(m, n)$ (recall that the initial solution is $\mathcal{A} = \emptyset$). Due to the URP assumption, $\mathcal{E}_{\mathcal{B}} = \mathcal{E}_{\mathcal{A}} = \min_{\mathbf{x} \in \mathbb{R}^n} \mathcal{E}(\mathbf{x})$ is the optimal least-square cost. Therefore, $\|\mathcal{A}\|_0 > \|\mathcal{B}\|_0 \Rightarrow \forall \lambda > 0, \mathcal{J}_{\mathcal{A}}(\lambda) > \mathcal{J}_{\mathcal{B}}(\lambda)$. This cannot occur because SBR is a descent algorithm.

— CSBR. Recursively, for each $\lambda = \lambda_q$, if the initial set \mathcal{A}_{q-1} (input of $SBR(\lambda_q)$) is of cardinality lower than $\min(m, n)$, then the output \mathcal{A}_q of $SBR(\lambda_q)$ is also of cardinality lower than $\min(m, n)$.

4.3 Termination of CSBR

Remark 9 When CSBR terminates, $\mathcal{E}_{\mathcal{A}} = \mathcal{J}_{\mathcal{A}}(0)$ is locally minimum w.r.t. \mathcal{A} , then $\forall i \notin \mathcal{A}, \mathcal{E}_{\mathcal{A} \cup i} = \mathcal{E}_{\mathcal{A}}$.

Remark 10 CSBR terminates after a finite number of SBR iterations.

Proof 18 • According to remark 4, for a given λ -value λ_q , $SBR(\lambda_q)$ terminates after a finite number of iterations.

- According to remark 7, each value of λ_q is such that there exists $\underline{\mu}_q$ and $\overline{\mu}_q$ such that

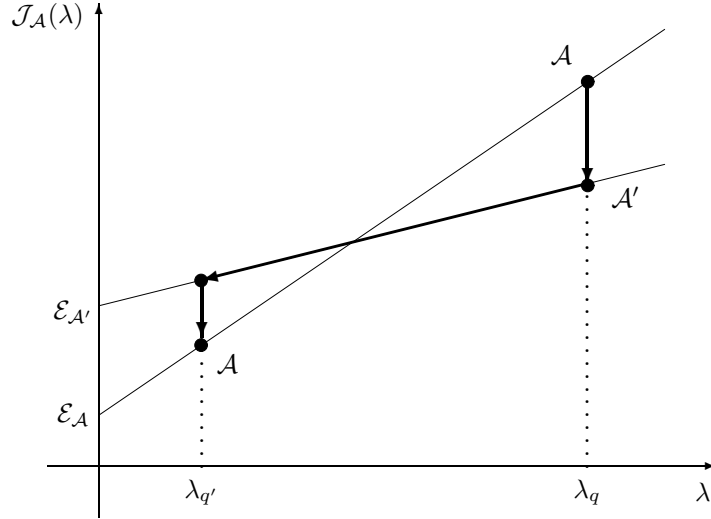


Figure 3: A given set \mathcal{A} may be explored twice during the CSBR procedure, at different λ -values. Here, each vertical line corresponds to one call to SBR (\mathcal{A} and \mathcal{A}' are two SBR iterates at λ_q and $\lambda_{q'}$), *i.e.*, to a fixed λ -value while the plain lines are the affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{A}'}(\lambda)$.

- $0 \leq \underline{\mu}_q \leq \lambda_q \leq \overline{\mu}_q$;
- $\lambda_q = (\underline{\mu}_q + \overline{\mu}_q)/2$;
- $\underline{\mu}_q$ and $\overline{\mu}_q$ are critical values for which two affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda \cup i)$ intersect.

From the recursive construction of the sequence $(\lambda_q, q \geq 0)$, it is clear that $\forall q, \overline{\mu}_q < \lambda_{q-1}$, thus $\forall q, \overline{\mu}_q < \overline{\mu}_{q-1}$. Since each value of $\overline{\mu}_q$ can be associated to a given intersection between two affine curves $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda)$ and $\lambda \mapsto \mathcal{J}_{\mathcal{B}}(\lambda)$ and the number of possible subsets \mathcal{A} and \mathcal{B} of $\{1, \dots, n\}$ whose cardinality is lower than $\min(m, n)$ is finite, the number of possible values taken by $\overline{\mu}_q$ is also finite. Since the sequence $(\overline{\mu}_q, q \geq 0)$ satisfies $\forall q, \overline{\mu}_q < \overline{\mu}_{q-1}$, we conclude that the number of iterations q at which SBR(λ_q) is run is finite.

Despite remark 10, we cannot claim that a given set \mathcal{A} is never explored twice during the CSBR procedure. In remark 4, we have seen that a given set \mathcal{A} can never be explored twice while running SBR for a given λ -value. However, \mathcal{A} may be explored several times while running CSBR, *i.e.*, once while running SBR at some λ -value λ_q , and another time while running SBR at another λ -value $\lambda_{q'} \leq \lambda_q$ (for $q' > q$). See Fig. 3 for a simple illustration.

Remark 11 When CSBR terminates, the solution $\mathbf{x}_{\mathcal{A}}$ is an unconstrained least-square estimate.

Proof 19 Let us define the residual $\mathbf{r} = \mathbf{y} - \mathbf{A}\mathbf{x}_{\mathcal{A}}$ and the unit vectors $\mathbf{e}_i \in \mathbb{R}^n$ in which all entries are equal to 0 except the i -th entry, equal to 1. Then, $\mathbf{A}\mathbf{e}_i = \mathbf{a}_i$, where \mathbf{a}_i stands for the i -th column of \mathbf{A} .

Firstly, we prove that $\forall i \notin \mathcal{A}, \mathbf{a}_i^T \mathbf{r} = 0$. According to remark 9, \mathcal{A} is such that $\forall i \notin \mathcal{A}, \mathcal{E}_{\mathcal{A} \cup i} = \mathcal{E}_{\mathcal{A}}$. Then, the following inequalities hold:

$$\begin{aligned}
 \forall i \notin \mathcal{A}, \quad \forall \varepsilon \in \mathbb{R}, \quad \mathcal{E}(\mathbf{x}_{\mathcal{A}} + \varepsilon \mathbf{e}_i) - \mathcal{E}(\mathbf{x}_{\mathcal{A}}) &\geq 0 \\
 \forall i \notin \mathcal{A}, \quad \forall \varepsilon \in \mathbb{R}, \quad \|\mathbf{r} - \varepsilon \mathbf{a}_i\|^2 - \|\mathbf{r}\|^2 &\geq 0 \\
 \forall i \notin \mathcal{A}, \quad \forall \varepsilon \in \mathbb{R}, \quad \varepsilon^2 \|\mathbf{a}_i\|^2 - 2\varepsilon \mathbf{a}_i^T \mathbf{r} &\geq 0 \\
 \forall i \notin \mathcal{A}, \quad \mathbf{a}_i^T \mathbf{r} &= 0.
 \end{aligned}$$

Secondly, because $\mathbf{x}_{\mathcal{A}}$ is a solution to the constrained problem (2):

$$\begin{aligned} \forall i \in \mathcal{A}, \quad \forall \varepsilon \in \mathbb{R}, \quad \mathcal{E}(\mathbf{x}_{\mathcal{A}} + \varepsilon \mathbf{e}_i) - \mathcal{E}(\mathbf{x}_{\mathcal{A}}) &\geq 0 \\ \forall i \in \mathcal{A}, \quad \mathbf{a}_i^T \mathbf{r} &= 0. \end{aligned}$$

Finally, we deduce that

$$\begin{aligned} \forall i \in \{1, \dots, n\}, \quad \mathbf{a}_i^T \mathbf{r} &= 0 \\ \mathbf{A}^T \mathbf{r} &= \mathbf{0} \\ \mathbf{A}^T \mathbf{A} \mathbf{x}_{\mathcal{A}} - \mathbf{A}^T \mathbf{y} &= \mathbf{0} \\ \nabla \mathcal{E}(\mathbf{x}_{\mathcal{A}}) &= \mathbf{0}. \end{aligned}$$

Since \mathcal{E} is quadratic, we have shown that $\mathbf{x}_{\mathcal{A}}$ is an unconstrained least-square estimate.

References

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