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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  $\mathcal{D}_k \subset \mathbb{R}^n$ :

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

**Theorem 1** For  $k \ge 1$ ,  $\mathcal{D}_k$  is not a closed set, and  $\overline{\mathcal{D}_k} = \{ x \in \mathbb{R}^n, \|x\|_0 \le k \}$  (denoting by – 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  $\mathbf{0} \notin \mathcal{D}_k$ .
  - $\overline{\mathcal{D}_k} \subseteq \{ \boldsymbol{x} \in \mathbb{R}^n, \| \boldsymbol{x} \|_0 \leq k \}$ . If  $\boldsymbol{x} \in \overline{\mathcal{D}_k}$ , then there exists a sequence  $\boldsymbol{x}_j \in \mathcal{D}_k \ (j \in \mathbb{N})$  whose limit is equal to  $\boldsymbol{x}$ . Then,

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

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

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

The consequence of theorem 1 is that

$$rgmin_{oldsymbol{x}\in\mathcal{D}_k} \left\{\mathcal{E}(oldsymbol{x}) = \|oldsymbol{y}-oldsymbol{A}oldsymbol{x}\|^2
ight\}$$

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

$$\mathcal{X}_{c}(k) = \operatorname*{arg\,min}_{\boldsymbol{x} \in \overline{\mathcal{D}_{k}}} \, \mathcal{E}(\boldsymbol{x}) = \operatorname*{arg\,min}_{\|\boldsymbol{x}\|_{0} \leqslant k} \, \mathcal{E}(\boldsymbol{x})$$

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  $\|\boldsymbol{x}\|^2$  over the domain  $\mathcal{D}_k$ . For  $k \ge 1$ , there is no minimizer over  $\mathcal{D}_k$ , but the minimal cost  $\min_{\boldsymbol{x}\in\mathcal{D}_k} \|\boldsymbol{x}\|^2$  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  $\mathcal{E}(\boldsymbol{x}) = \boldsymbol{x}(1)^2$ . It is easy to see that  $\mathcal{X}_c(0) = \{\mathbf{0}\}, \ \mathcal{X}_c(1) = \{[0, \boldsymbol{x}(2)]^T, \ \boldsymbol{x}(2) \in \mathbb{R}\}$  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

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

**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 A of size  $m \times n$  ( $m \leq n$ ) satisfies the URP if and only if any selection of m columns of A forms a family of linearly independent vectors.

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

When m > n, we adopt the following definition:

**Definition 2** A matrix 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  $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$  but the minimizer of  $\mathcal{E}(\boldsymbol{x})$  over  $\mathbb{R}^n$  is unique (although not necessarily sparse):  $\mathcal{X}_c(n) = \{(\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{A}^T \boldsymbol{y}\}.$ 

In the following, we will assume that  $y \neq 0$  and that 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 A yields a matrix 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 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  $\mathcal{X}_c(k)$ ,  $k = 0, \ldots, n$  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  $\mathcal{A}(\mathbf{x}_m) \subset \mathcal{B} \subseteq \{1, \ldots, n\}$ , 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  $\mathcal{E}(\mathbf{x}_m + \mathbf{n}) = \mathcal{E}(\mathbf{x}_m) = \max_{\mathbf{x} \in \mathbb{R}^n} \mathcal{E}(\mathbf{x})$ . 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  $(m \le n \text{ or } m > n)$ . 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  $\lambda \ge 0$ , we define the set of minimizers of  $\mathcal{J}(\boldsymbol{x};\lambda) = \mathcal{E}(\boldsymbol{x}) + \lambda \|\boldsymbol{x}\|_0$ :

$$\mathcal{X}_p(\lambda) = \operatorname*{arg\,min}_{oldsymbol{x} \in \mathbb{R}^n} \left\{ \mathcal{J}(oldsymbol{x}; \lambda) 
ight\}$$

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

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

$$\|\mathcal{A}\|_{0} \triangleq Card(\mathcal{A})$$

**Definition 5** We denote by  $\mathcal{A}(\mathbf{x}) \subseteq \{1, \ldots, n\}$  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

$$\boldsymbol{x}_{\mathcal{A}} \triangleq \underset{\mathcal{A}(\boldsymbol{x}) \subseteq \mathcal{A}}{\operatorname{arg\,min}} \mathcal{E}(\boldsymbol{x}) \tag{2}$$

and the corresponding least-square cost by

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

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

$$\mathcal{J}_{\mathcal{A}}(\lambda) \triangleq \mathcal{J}(\boldsymbol{x}_{\mathcal{A}};\lambda) = \mathcal{E}_{\mathcal{A}} + \lambda \|\boldsymbol{x}_{\mathcal{A}}\|_{0}$$
(4)

which is generally different from

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

**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

$$oldsymbol{x}_p(\lambda) \in rgmin_{\{oldsymbol{x} \in \mathbb{R}^n, \, \mathcal{A}(oldsymbol{x}) \subseteq \mathcal{A}\}} \mathcal{E}(oldsymbol{x})$$

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

$$egin{aligned} \mathcal{J}(m{x};\lambda) & \geqslant & \mathcal{J}(m{x}_p(\lambda);\lambda) \ \mathcal{E}(m{x})+\lambda\|m{x}\|_0 & \geqslant & \mathcal{E}(m{x}_p(\lambda))+\lambda\|\mathcal{A}\|_0 \ \mathcal{E}(m{x})-\mathcal{E}(m{x}_p(\lambda)) & \geqslant & \lambdaig(\|\mathcal{A}\|_0-\|m{x}\|_0ig) \geqslant 0 \end{aligned}$$

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

- 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  $\{x \in \mathbb{R}^n, \mathcal{A}(x) \subseteq \mathcal{A}\}$  (URP assumption), which is  $x_{\mathcal{A}}$ .

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

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  $\lambda \ge 0$ ) guarantees that  $\mathcal{X}_p(\lambda)$  is of finite cardinality for all  $\lambda$ . 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  $\sum_{k=0}^{\min(m,n)} C_n^k$ :  $\{ \mathbf{x} \in \mathbb{R}^n, \exists A \subseteq \{1,\ldots,n\}, \|A\|_0 \le \min(m,n) \text{ and } \mathbf{x} = \mathbf{x}_A \}$ .

#### 3.2 Piecewise constant property

**Theorem 6** The dependence of the set  $\mathcal{X}_p(\lambda)$  w.r.t.  $\lambda$  ( $\lambda > 0$ ) 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  $\lambda$ , and

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

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

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

 $\lambda_i^*$  are also the  $\lambda$ -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  $\lambda$  is fixed, let  $\boldsymbol{x}_p(\lambda) \in \mathcal{X}_p(\lambda)$ , and let  $\mathcal{A} \triangleq \mathcal{A}(\boldsymbol{x}_p(\lambda))$ .

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

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

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

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

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

 $\lambda \mapsto \mathcal{J}(\lambda)$  is a continuous and piecewise linear function of  $\lambda$  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  $\lambda_i^* (i = 1, \dots, I)$  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:

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

$$\tag{7}$$

In particular, for i = 0, we have

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

where  $\mathcal{E}_{\mathcal{A}_0} = \min_{\boldsymbol{x} \in \mathbb{R}^n} \mathcal{E}(\boldsymbol{x})$  is the minimal least-square error, and  $\|\boldsymbol{x}_{\mathcal{A}_0}\|_0$  is the minimal L0-norm of the minimizers of  $\mathcal{E}$  over  $\mathbb{R}^n$ . For i = I, we have necessarily  $\boldsymbol{x}_{\mathcal{A}_I} = \mathbf{0}$  and  $\mathcal{E}_{\mathcal{A}_I} = \|\boldsymbol{y}\|^2$ , thus

$$\forall \lambda \in [\lambda_I^*, +\infty), \ \mathcal{J}(\lambda) = \|\boldsymbol{y}\|^2.$$
(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  $\lambda$ -value  $\in (\lambda_i^*, \lambda_{i+1}^*)$ , we consider  $\mathbf{x} \in \mathcal{X}_p(\lambda)$ , then necessarily, the following equivalent equations hold:

$$egin{array}{rcl} \mathcal{J}(\lambda) &=& \mathcal{J}(oldsymbol{x};\lambda) \ \mathcal{E}_{\mathcal{A}_i}+\lambda\|oldsymbol{x}_{\mathcal{A}_i}\|_0 &=& \mathcal{E}(oldsymbol{x})+\lambda\|oldsymbol{x}\|_0 \end{array}$$

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  $m \ge n$ , 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  $m \ge n$ ,  $\mathcal{X}_p(0)$  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  $(I \ge 1)$ , thus  $\mathcal{X}_p(0) \subset \mathcal{X}_p$ .

**Theorem 7** For a given  $\lambda$ -value which is distinct from  $\lambda_0^*, \lambda_1^*, \ldots, \lambda_I^*$ , all the elements of  $\mathcal{X}_p(\lambda)$  are of same L0-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  $A_i \subseteq \{1, \ldots, n\}$  such that

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

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

$$\forall \lambda' \in [\lambda_i^{\star}, \lambda_{i+1}^{\star}], \ \mathcal{J}(\boldsymbol{x}_p(\lambda); \lambda') = \mathcal{J}_{\mathcal{A}_i}(\lambda')$$
  
$$\forall \lambda' \in [\lambda_i^{\star}, \lambda_{i+1}^{\star}], \ \mathcal{E}(\boldsymbol{x}_p(\lambda)) + \lambda' \| \boldsymbol{x}_p(\lambda) \|_0 = \mathcal{E}_{\mathcal{A}_i} + \lambda' \| \boldsymbol{x}_{\mathcal{A}_i} \|_0.$$
(11)

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

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

**Proof 11** • Recall that for  $i \in \{0, ..., I\}$ , 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:  $\forall \lambda \notin \{\lambda_0^*, \dots, \lambda_I^*\}, \|\boldsymbol{x}_p(\lambda)\|_0 = \mathcal{J}'(\lambda)$ , and of lemma 1:  $\mathcal{J}$  is a concave function, thus its derivative (when it is defined) is a decreasing function of  $\lambda$ . At this point, we know that  $\lambda \mapsto \|\boldsymbol{x}_p(\lambda)\|_0$  is piecewise constant on  $\mathbb{R}_+$ , and that its restriction to  $\mathbb{R}_+ \setminus \{\lambda_0^*, \dots, \lambda_I^*\}$  is decreasing:  $\forall i \in \{1, \dots, I\}, \|\boldsymbol{x}_{\mathcal{A}_{i-1}}\|_0 \ge \|\boldsymbol{x}_{\mathcal{A}_i}\|_0$ . The remaining part is to study the behavior of  $\|\boldsymbol{x}_p(\lambda)\|_0$ at  $\lambda = \lambda_i^*, i = 0, \dots, I$ .

For  $i \in \{1, \ldots, I\}$ , let us show that  $\boldsymbol{x}_p(\lambda_i^{\star})$  is such that  $\|\boldsymbol{x}_{\mathcal{A}_{i-1}}\|_0 \ge \|\boldsymbol{x}_p(\lambda_i^{\star})\|_0 \ge \|\boldsymbol{x}_{\mathcal{A}_i}\|_0$ :

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

Due to the definition of  $\lambda \mapsto \mathcal{J}(\lambda)$  in theorem 6, the affine function  $\lambda \mapsto \mathcal{J}(\boldsymbol{x}_p(\lambda_i^*);\lambda)$  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  $\|\boldsymbol{x}_{\mathcal{A}_{i-1}}\|_0 \geq \|\boldsymbol{x}_p(\lambda_i^*)\|_0 \geq \|\boldsymbol{x}_{\mathcal{A}_i}\|_0$ .

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

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

• Second result: for a given  $i \in \{1, \ldots, I\}$ , the continuity of  $\mathcal{J}$  at  $\lambda = \lambda_i^{\star}$  reads  $\mathcal{E}_{\mathcal{A}_{i-1}} + \lambda_i^{\star} \| \boldsymbol{x}_{\mathcal{A}_{i-1}} \|_0 = \mathcal{E}_{\mathcal{A}_i} + \lambda_i^{\star} \| \boldsymbol{x}_{\mathcal{A}_i} \|_0$ . Because  $\| \boldsymbol{x}_{\mathcal{A}_{i-1}} \|_0 \ge \| \boldsymbol{x}_{\mathcal{A}_i} \|_0$ ,  $\mathcal{E}_{\mathcal{A}_{i-1}} \le \mathcal{E}_{\mathcal{A}_i}$ .

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

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

It is easy to see that:

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

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

#### **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  $\lambda \neq \{\lambda_0^{\star}, \ldots, \lambda_I^{\star}\}$ , then there exists k such that  $\mathcal{X}_p(\lambda) = \mathcal{X}_c(k)$ .

**Proof 12** For a given  $\lambda$ -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

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

or equivalently,

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

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

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



Figure 1: Representation of the affine curves  $\lambda \mapsto \mathcal{J}_{\mathcal{A}}(\lambda) = \mathcal{E}_{\mathcal{A}} + \lambda \| \boldsymbol{x}_{\mathcal{A}} \|_{0}$  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  $\lambda \mapsto \mathcal{J}_{\mathcal{A}_{1}}(\lambda)$ ) for which  $\| \boldsymbol{x}_{\mathcal{A}} \|_{0}$  is equal to 3, 2 and 0, respectively.  $\mathcal{A}'_{1}$  is an active set such that  $\| \boldsymbol{x}_{\mathcal{A}'_{1}} \|_{0} = 2$  but  $\mathcal{E}_{\mathcal{A}'_{1}} > \mathcal{E}_{\mathcal{A}_{1}}$ . No active set such that  $\| \boldsymbol{x}_{\mathcal{A}} \|_{0} = 1$  is present in  $\mathcal{X}_{p}$ .  $\mathcal{B}$  is the active set such that  $\| \boldsymbol{x}_{\mathcal{B}} \|_{0} = 1$  whose energy  $\mathcal{E}_{\mathcal{B}}$  is the lowest among all the active sets such that  $\| \boldsymbol{x}_{\mathcal{A}} \|_{0} \leq 1$ , however,  $\forall \lambda, \mathcal{J}_{\mathcal{B}}(\lambda) > \mathcal{J}(\lambda)$ . Thus,  $\mathcal{X}_{c}(1) = \{ \boldsymbol{x}_{\mathcal{B}} \} \not\subset \mathcal{X}_{p}$ . On the contrary, for all  $\lambda \neq \{ \lambda_{0}^{*}, \dots, \lambda_{I}^{*} \}, \mathcal{X}_{p}(\lambda) = \mathcal{X}_{c}(k_{\lambda})$ , with  $k_{\lambda} = \mathcal{J}'(\lambda) = 3, 2$  or 0.



Figure 2: Content of  $\mathcal{X}_p(\lambda)$  at a critical  $\lambda$ -value  $\lambda = \lambda_i^*, i \ge 1$ :  $\mathcal{X}_p(\lambda_i^*) \subset \mathcal{X}_c$ , and  $Card(\mathcal{X}_p(\lambda_i^*)) \ge 2$ . On this example,  $\mathcal{X}_p(\lambda_2^*) = \mathcal{X}_c(0) \cup \mathcal{X}_c(1) \cup \mathcal{X}_c(2)$  and  $Card(\mathcal{X}_p(\lambda_2^*)) \ge 3$  since  $\mathbf{x}_{\mathcal{A}_1}, \mathbf{x}_{\mathcal{A}_2}$  and  $\mathbf{x}_{\mathcal{B}} \in \mathcal{X}_p(\lambda_2^*)$ .

- Now, let us prove the reverse inclusion. Given  $\lambda$ , 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

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

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

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

**Lemma 3** If  $\lambda_{i-1}^{\star} < \lambda < \lambda_i^{\star} < \lambda' < \lambda_{i+1}^{\star}$ , 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 L0-norm, which is the derivative of  $\mathcal{J}$  at  $\lambda$  (resp.  $\lambda'$ ). 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  $\lambda_i^*$  (critical point, at which the derivative of  $\mathcal{J}$  is changing).

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

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  $Card(\mathcal{X}_p(\lambda)) + Card(\mathcal{X}_p(\lambda')) \leq Card(\mathcal{X}_p(\lambda_i^*))$ .
  - 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  $Card(\mathcal{X}_p(\lambda)) + Card(\mathcal{X}_p(\lambda')) \leq Card(\mathcal{X}_p(\lambda^*_i))$ , we deduce that  $Card(\mathcal{X}_p(\lambda)) < Card(\mathcal{X}_p(\lambda^*_i))$ and  $Card(\mathcal{X}_p(\lambda')) < Card(\mathcal{X}_p(\lambda^*_i))$ .

### 4 SBR and CSBR algorithms

#### 4.1 SBR iterates and output

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

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

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

First, recall that for the SBR iterates (and in particular when SBR terminates),  $\|\boldsymbol{x}_{\mathcal{A}}\|_0 = \|\mathcal{A}\|_0$ . 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  $\boldsymbol{x}_{\mathcal{A}}(i) = 0$  (however, these removals rarely occur in practice). The following remark follows from this property.

**Remark 3** For a given  $\lambda$ -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 A which are reachable is finite (i.e., the number of subsets of  $\{1, \ldots, n\}$ ).

**Remark 5** When SBR terminates, the estimate  $\hat{x}(\lambda) = x_A$  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  $\bullet \triangleq \cup \text{ or } \setminus$ ) does not yield a decrease of the cost  $\mathcal{J}_{\mathcal{A}}(\lambda)$ ). Formally, this property reads:

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

or equivalently,

$$\forall i, \, \mathcal{E}_{\mathcal{A}} + \lambda \|\mathcal{A}\|_{0} \leq \mathcal{E}_{\mathcal{A} \bullet i} + \lambda \|\boldsymbol{x}_{\mathcal{A} \bullet i}\|_{0} \forall i, \, \mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \bullet i} \leq \lambda (\|\boldsymbol{x}_{\mathcal{A} \bullet i}\|_{0} - \|\mathcal{A}\|_{0}).$$

$$(13)$$

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

When  $\bullet = \backslash$ , both terms on the left- and right-hand sides of the inequality are strictly negative  $(\|\boldsymbol{x}_{\mathcal{A}\backslash i}\|_0 \leq \|\mathcal{A}\|_0 - 1)$ , 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  $\|\boldsymbol{x}_{\mathcal{A}\cup i}\|_0 = \|\mathcal{A}\|_0$  or  $\|\mathcal{A}\|_0 + 1$ ). Therefore, (13) remains valid for  $\lambda \neq \lambda_q$  if and only if

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

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

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

How to choose  $\lambda_{q+1}$ ? Setting  $\lambda_{q+1}$  to the lower bound of (15) is not judicious, since for this  $\lambda$ -value,  $\mathcal{J}$  is still "locally minimum w.r.t.  $\mathcal{A}$ " in the sense of (12). One possibility is to set  $\lambda_{q+1}$  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

$$\widetilde{\lambda}_i \triangleq \mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \cup i} \ge 0 \tag{16}$$

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

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

**Remark 7** For a given  $i \notin \mathcal{A}$  for which  $\|\boldsymbol{x}_{\mathcal{A}\cup i}\|_0 = \|\mathcal{A}\|_0 + 1$ ,  $\lambda_i$  is the  $\lambda$ -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

$$\widetilde{\lambda}_{i} \triangleq \frac{\mathcal{E}_{\mathcal{A}} - \mathcal{E}_{\mathcal{A} \setminus i}}{\|\boldsymbol{x}_{\mathcal{A} \setminus i}\|_{0} - \|\mathcal{A}\|_{0}}$$
(17)

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

**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,  $\mathcal{E}_{\mathcal{B}} = \mathcal{E}_{\mathcal{A}} = \min_{\boldsymbol{x} \in \mathbb{R}^n} \mathcal{E}(\boldsymbol{x})$  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  $\lambda$ -value  $\lambda_q$ ,  $SBR(\lambda_q)$  terminates after a finite number of *iterations.* 
  - According to remark 7, each value of  $\lambda_q$  is such that there exists  $\mu_q$  and  $\overline{\mu_q}$  such that



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

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

From the recursive construction of the sequence  $(\lambda_q, q \ge 0)$ , 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  $\{1, \ldots, n\}$  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  $(\overline{\mu_q}, q \ge 0)$  satisfies  $\forall q, \overline{\mu_q} < \overline{\mu_{q-1}}$ , we conclude that the number of iterations q at which  $SBR(\lambda_q)$  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  $\lambda$ -value. However,  $\mathcal{A}$  may be explored several times while running CSBR, *i.e.*, once while running SBR at some  $\lambda$ -value  $\lambda_q$ , and another time while running SBR at another  $\lambda$ -value  $\lambda_{q'} \leq \lambda_q$  (for q' > q). See Fig. 3 for a simple illustration.

**Remark 11** When CSBR terminates, the solution  $x_A$  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  $\forall i \notin \mathcal{A}$ ,  $a_i^T r = 0$ . 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:

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

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

$$\forall i \in \mathcal{A}, \quad \forall \varepsilon \in \mathbb{R}, \ \mathcal{E}(\boldsymbol{x}_{\mathcal{A}} + \varepsilon \boldsymbol{e}_{i}) - \mathcal{E}(\boldsymbol{x}_{\mathcal{A}}) \ge 0 \\ \forall i \in \mathcal{A}, \quad \boldsymbol{a}_{i}^{T} \boldsymbol{r} = 0.$$

Finally, we deduce that

$$orall i \in \{1, \dots, n\}, \ oldsymbol{a}_i^T oldsymbol{r} = 0$$
  
 $oldsymbol{A}^T oldsymbol{r} = oldsymbol{0}$   
 $oldsymbol{A}^T oldsymbol{A} oldsymbol{a}_{\mathcal{A}} - oldsymbol{A}^T oldsymbol{y} = oldsymbol{0}$   
 $abla \mathcal{E}(oldsymbol{x}_{\mathcal{A}}) = oldsymbol{0}.$ 

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

## References

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