

The Geometry of Uniqueness, Sparsity and Clustering in Penalized Estimation

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Abstract

We provide a necessary and sufficient condition for the uniqueness of penalized least-squares estimators whose penalty term is given by a norm with a polytope unit ball, covering a wide range of methods including SLOPE, PACS, fused, clustered and classical LASSO as well as the related method of basis pursuit. We consider a strong type of uniqueness that is relevant for statistical problems. The uniqueness condition is geometric and involves how the row span of the design matrix intersects the faces of the dual norm unit ball, which for SLOPE is given by the signed permutahedron. Further considerations based this condition also allow to derive results on sparsity and clustering features. In particular, we define the notion of a SLOPE pattern to describe both sparsity and clustering properties of this method and also provide a geometric characterization of accessible SLOPE patterns.

Keywords: Penalized Estimation, SLOPE, Uniqueness, Sparsity, Clustering, Regularization, Geometry, Polytope

1. Introduction

The linear regression model $Y = X\beta + \varepsilon$, where $X \in \mathbb{R}^{n \times p}$ is a fixed matrix, $\beta \in \mathbb{R}^p$ is an unknown parameter vector, and ε is a centered random error term in \mathbb{R}^n , plays a central role in statistics. When $\ker(X) = \{0\}$, the ordinary least-squares estimator $\hat{\beta}^{\text{ols}} = (X'X)^{-1}X'Y$, which minimizes the residual sum of squares $\|Y - Xb\|_2^2$ with respect to $b \in \mathbb{R}^p$, is the usual estimator of β . In high dimensions, when $p > n$, and thus $\ker(X) \neq \{0\}$, the ordinary least squares estimator is no longer well-defined, as then the function $b \in \mathbb{R}^p \mapsto \|Y - Xb\|_2^2$ does not have a unique minimizer.

In this case, typically, a penalty term is added to the residual sum of squares to provide an alternative to ordinary least-squares estimation. In some cases, also the minimizer of the penalized least-squares optimization problem is not unique. Since Y is a random vector and the induced stochastic properties on the minimizer are often the object of study in a statistical framework, it is relevant to consider a strong type of uniqueness: uniqueness for

a given X that holds for all realizations¹ of Y in \mathbb{R}^n . In this paper, we provide a necessary and sufficient condition for uniqueness for a wide class of penalties based on a geometric criterion, as well as for the related methods of basis pursuit. Moreover, the geometry involved in this condition also yields results for model selection and pattern recovery, i.e., sparsity and related clustering properties, which we investigate for SLOPE in particular.

1.1 Penalized least-squares estimators and uniqueness

The Ridge estimator, minimizing the function $b \in \mathbb{R}^p \mapsto \frac{1}{2} \|Y - Xb\|_2^2 + \lambda \|b\|_2^2$, where $\lambda > 0$ is a tuning parameter, was the first penalized estimator to appear in the statistics literature (Hoerl and Kennard, 1970; Golub et al., 1979). Due to the strict convexity of the function $b \mapsto \|b\|_2^2$, the minimizer is always unique and given by $\hat{\beta}^{\text{ridge}} = (X'X + \lambda \mathbb{I}_p)^{-1} X'Y$. This estimator is not sparse, meaning that it does not set components equal to zero almost surely. Especially when p is large, this can make the estimator more difficult to interpret compared to other methods such as LASSO or SLOPE, which do exhibit sparsity and are described in the following.

The Least Absolute Shrinkage and Selection Operator or LASSO (Chen and Donoho, 1994; Alliney and Ruzinsky, 1994; Tibshirani, 1996) is the ℓ_1 -penalized least-squares estimator defined as

$$\hat{\beta}^{\text{lasso}} = \arg \min_{b \in \mathbb{R}^p} \frac{1}{2} \|Y - Xb\|_2^2 + \lambda \|b\|_1, \text{ where } \lambda > 0.$$

When $\ker(X) = \{0\}$, the function $b \in \mathbb{R}^p \mapsto \|Y - Xb\|_2^2$ is strictly convex, immediately implying the uniqueness of the LASSO minimizer. In high dimensions, $\ker(X) \neq \{0\}$ and the function $b \in \mathbb{R}^p \mapsto \|Y - Xb\|_2^2$ is not strictly convex, thus uniqueness of $\hat{\beta}^{\text{lasso}}$ is not guaranteed. A geometric description of the set of LASSO minimizers, relevant when non-uniqueness occurs, is given in Dupuis and Vaiter (2019). A sufficient condition for uniqueness of the estimator for all $Y \in \mathbb{R}^n$ is for the columns of the design matrix X to be in general position. This was first outlined by Rosset et al. (2004) and later investigated by Tibshirani (2013) and Ali and Tibshirani (2019). Recently, this condition was relaxed by Ewald and Schneider (2020) to a geometric criterion that is both sufficient and necessary and which is generalized for a wide class of possible penalty terms in the present paper.

A strongly related procedure is basis pursuit, which first appeared in compressed sensing (Chen and Donoho, 1994) and is defined as

$$\hat{\beta}^{\text{bp}} = \arg \min \|b\|_1 \text{ subject to } Y = Xb,$$

provided that $Y \in \text{col}(X)$. In the noiseless case, this method allows to recover a sparse vector β (see e.g. Candès et al., 2006; Cohen et al., 2009). In the noisy case, when ε is no longer zero, the basis pursuit estimator can be viewed as the LASSO when the tuning parameter $\lambda > 0$ becomes infinitely small (Dossal, 2012, Lemma 3.6)². Naturally, basis

1. Certain results in the literature (Zhang et al., 2015; Gilbert, 2017; Mousavi and Shen, 2019) provide a criterion for the uniqueness of a given minimizer. These results naturally differ strongly from the ones in the present article as they deal with a weaker notion of uniqueness.
 2. This reference focuses on necessary and sufficient conditions to uniquely recover a given b_0 from $y = Xb_0$ (in our notation), which is a different type of uniqueness than we consider.

pursuit shares a lot of properties with the LASSO estimator. For example, general position of the columns of the design matrix X is also a sufficient condition for uniqueness of $\hat{\beta}^{\text{bp}}$ for all $Y \in \mathbb{R}^n$ (see e.g. Dossal, 2012). However, to the best of our knowledge, a necessary and sufficient condition for this type of uniqueness has previously been unknown.

Our results also cover Sorted L-One Penalized Estimation or SLOPE (Bogdan et al., 2015; Negrinho and Martins, 2014; Zeng and Figueiredo, 2014), which is the penalized estimator given by

$$\hat{\beta}^{\text{slope}} = \arg \min_{b \in \mathbb{R}^p} \frac{1}{2} \|Y - Xb\|_2^2 + \sum_{j=1}^p w_j |b|_{(j)},$$

where $w_1 > 0$, $w_1 \geq \dots \geq w_p \geq 0$, and $|b|_{(1)} \geq \dots \geq |b|_{(p)}$. Note that the penalty term gives rise to the so-called sorted- ℓ_1 -norm. A special case of this estimator, the Octagonal Shrinkage and Clustering Algorithm for Regression or OSCAR, has already been introduced in Bondell and Reich (2008). The SLOPE estimator is well-defined once the corresponding minimizer is unique and, similarly to the LASSO, uniqueness is obvious when $\ker(X) = \{0\}$. However, in contrast to the LASSO, no condition guaranteeing uniqueness has previously been established.

1.2 Uniqueness and polytope unit balls

In this paper, we study the problem of uniqueness of penalized estimators in a general setting, where the penalty term is not restricted the ℓ_1 - or the sorted- ℓ_1 -norm. We describe the framework we consider in the following. Let $X \in \mathbb{R}^{n \times p}$, $y \in \mathbb{R}^n$, and $\|\cdot\|$ be a norm on \mathbb{R}^p . Consider the solution set $S_{X, \|\cdot\|}(y)$ to the penalized least-squares problem

$$S_{X, \|\cdot\|}(y) = \text{Arg} \min_{b \in \mathbb{R}^p} \frac{1}{2} \|y - Xb\|_2^2 + \|b\|.$$

Note that $S_{X, \|\cdot\|}(y)$ is non-empty since the function $b \in \mathbb{R}^p \mapsto \frac{1}{2} \|y - Xb\|_2^2 + \|b\|$ is continuous and unbounded when $\|b\|$ becomes large. The penalty term may include a positive tuning parameter which can be viewed as part of the norm, for instance $\|\cdot\| = \lambda \|\cdot\|_1$ for the LASSO estimator. When $\|\cdot\|$ is a norm for which $\|b + \tilde{b}\| = \|b\| + \|\tilde{b}\|$ holds if and only if $b = t\tilde{b}$ where $t \geq 0^3$, such as the ℓ_2 -norm, then $S_{X, \|\cdot\|}(y)$ is a singleton for all $y \in \mathbb{R}^n$ and for all $X \in \mathbb{R}^{n \times p}$. This statement is a straightforward consequence of the following facts. When $\hat{\beta}, \tilde{\beta} \in S_{X, \|\cdot\|}(y)$ we have

- i) $X\hat{\beta} = X\tilde{\beta}$ (see Lemma 19 in the appendix).
- ii) Since $(\hat{\beta} + \tilde{\beta})/2 \in S_{X, \|\cdot\|}(y)$ also, $\|(\hat{\beta} + \tilde{\beta})/2\| = \|\hat{\beta}\| = \|\tilde{\beta}\| = (\|\hat{\beta}\| + \|\tilde{\beta}\|)/2$ follows.

Geometrically, such a norm $\|\cdot\|$ possesses a unit ball $\{x \in \mathbb{R}^p : \|x\| = 1\}$ with no edges. Subsequently, the problem of uniqueness is only relevant when the unit ball of the norm under consideration contains an edge. More concretely, we restrict our attention to norms for which the unit ball $B = \{x \in \mathbb{R}^p : \|x\| \leq 1\}$ is given by a polytope. Note that this

3. Typically, b and \tilde{b} are not orthogonal, thus the equality in the triangular inequality does not coincide with the decomposability property described in Negahban et al. (2012).

is the case for the ℓ_1 -norm, the ℓ_∞ -norm, and the sorted- ℓ_1 -norm. Our results also cover the fused LASSO (Tibshirani et al., 2005), the Pairwise Absolute Clustering and Sparsity (PACS) procedure (Sharma et al., 2013), the clustered LASSO (She, 2010), or methods with a mixed ℓ_1, ℓ_∞ -norm penalty term (Negahban and Wainwright, 2008; Bach et al., 2012).

1.3 Sparsity and clustering: accessible patterns and sign estimation

As mentioned above, the LASSO estimator is a sparse method that generally sets components equal to zero with positive probability, entailing that the estimator also performs so-called model or variable selection. In fact, when $p > n$ and the solution is unique, $\hat{\beta}^{\text{lasso}}$ contains at least $p - n$ zero components. Instigated by this property, an abundant literature has arisen to deal with the recovery of the location of the non-null components of β , or, more specifically, the recovery of the sign vector of β (Zou, 2006; Zhao and Yu, 2006; Wainwright, 2009).

A necessary condition for the recovery of $\text{sign}(\beta)$ is for this vector to be accessible by the LASSO, i.e., for a fixed $\lambda > 0$, there has to exist $Y \in \mathbb{R}^n$ for which $\text{sign}(\hat{\beta}^{\text{lasso}}) = \text{sign}(\beta)$. Otherwise, $\mathbb{P}(\text{sign}(\hat{\beta}^{\text{lasso}}) = \text{sign}(\beta)) = 0$, and recovery is clearly impossible. A geometrical characterization of accessible sign vectors is given in Sepehri and Harris (2017) under the assumption of uniqueness of LASSO solutions. In the appendix, we provide a geometrical characterization of accessible sign vectors for both basis pursuit and LASSO without a uniqueness assumption.

In the OSCAR procedure mentioned in Section 1.1, the letter ‘‘C’’ stands for ‘‘Clustering’’, referring to the fact that some components of this estimator can be equal in absolute value. This property can be illustrated for OSCAR – as well as the more general SLOPE method – by drawing the elliptic contour lines of the residual sum of squares $b \mapsto \|Y - Xb\|_2^2$ (when $\ker(X) = \{0\}$) together with balls of the sorted- ℓ_1 -norm⁴. This clustering property can also be deduced from the explicit expressions of SLOPE one obtains for the case where the columns of X are orthogonal (Tardivel et al., 2020; Dupuis and Tardivel, 2022). We show that the clustering phenomenon also holds in the general case by using our geometric approach. This feature of SLOPE – which is not shared by the LASSO – has, of course, been known in practice and may be of particular relevance in certain applications (Figueiredo and Nowak, 2016; Kremer et al., 2020, 2022).

With a similar objective as the articles written a decade ago on support or sign recovery by LASSO, there are now several papers dealing with pattern recovery by SLOPE where the notion of SLOPE pattern is a central concept (Skalski et al., 2022; Bogdan et al., 2022). In the present article, we show how our geometric approach can be used to provide a characterization of the clusters induced by SLOPE.

1.4 Related geometrical works

Most articles providing geometric properties in the context of penalized estimation treat the LASSO. Tibshirani and Taylor (2012) show that the LASSO residual $Y - X\hat{\beta}^{\text{lasso}}$ is the projection of Y onto the so-called LASSO null polyhedron $\{z \in \mathbb{R}^n : \|X'z\|_\infty \leq \lambda\}$. From this result, the authors derive an explicit formula for the Stein’s unbiased risk estimate that

4. See, e.g., Figure 2 in Bondell and Reich (2008) or Figure 1 in Zeng and Figueiredo (2014).

provides an unbiased estimator for $\mathbb{E}(\|X\hat{\beta}^{\text{lasso}} - X\beta\|_2^2)$. This geometric result also lays the groundwork for selective inference (Lee et al., 2016), for deriving screening procedures (Ghaoui et al., 2012; Wang et al., 2013), and to describe the accessible LASSO patterns in Sepehri and Harris (2017). For basis pursuit, geometrical considerations focus on dealing with the ℓ_1 -recovery in the noiseless case and are aimed at deriving the phase-transition curve (Donoho and Tanner, 2009). The recent article of Minami (2020) generalizes some results of Tibshirani and Taylor (2012) to SLOPE and shows that the number of non-null clusters (the quantity $\|\text{patt}(\hat{\beta}^{\text{slope}})\|_\infty$ in our article) appears in the Stein’s unbiased risk estimate for SLOPE estimator. For the sake of completeness we mention that in the present paper, we provide a convex null set in Proposition 11 that generalizes the concept of the LASSO null polyhedron to all norm-penalized least-squares estimators, where the projection of Y onto this set yields the estimation residuals.

1.5 Notation and structure

To conclude this section, we introduce the notation used throughout this article. We denote the set $\{1, \dots, k\}$ by $[k]$ and use $|I|$ for the cardinality of a set I . The set \mathcal{S}_p contains all permutations on the set $[p]$. For a matrix A , the symbols $\text{col}(A)$ and $\text{row}(A)$ stand for the column and row space of A , respectively, whereas $\text{conv}(A)$ represents the convex hull of the columns of A . As used in previous sections already, for a number t , $\text{sign}(t)$ is given by 1, -1 , or 0 if $t > 0$, $t < 0$, or $t = 0$, respectively. For a vector x , $\text{sign}(x)$ is the vector containing the signs of the components of x . Finally, the symbols $\|\cdot\|_1$, $\|\cdot\|_2$, $\|\cdot\|_\infty$, and $\|\cdot\|_w$ represent the ℓ_1 -, ℓ_2 -, supremum, and the sorted- ℓ_1 -norm, respectively.

The remainder of this article is organized as follows. Section 2 contains the main theorem of uniqueness for penalized least-squares estimators, as well as the analogous necessary and sufficient uniqueness condition for basis pursuit. In Section 3, we investigate the pattern selection properties related to the geometric condition introduced in Section 2 for SLOPE, including a characterization of the SLOPE’s clustering property. This section also contains a general result on the convex null set for norm-penalized least-squares estimation. Appendix A illustrates what our results entail for LASSO and BP. All proofs are relegated to Appendix B, which also contains a remainder of basic facts of subdifferentials and polytopes.

2. A necessary and sufficient condition for uniqueness of penalized problems

We start by providing the framework for the theorem on uniqueness of penalized least-squares minimization problems. For a norm $\|\cdot\|$ on \mathbb{R}^p , the dual norm $\|\cdot\|^*$ is defined by

$$\|x\|^* = \sup_{s \in \mathbb{R}^p: \|s\| \leq 1} s'x.$$

If the unit ball $B = \{x \in \mathbb{R}^p : \|x\| \leq 1\}$ is of polytope shape, the dual of B given by $B^* = \{x \in \mathbb{R}^p : \|x\|^* \leq 1\}$, the unit ball of the dual norm, is, again, a polytope. In this case, the penalty term is not differentiable everywhere and there is a strong connection between the subdifferentials $\partial_{\|\cdot\|}(\cdot)$ of the norm $\|\cdot\|$ and the faces of the polytope B^* . The precise association is detailed in Appendices B.1-B.3 and this connection provides the basis for the main theorem.

Theorem 1 (Necessary and sufficient condition for uniqueness) *Let $X \in \mathbb{R}^{n \times p}$ and let $\|\cdot\|$ be a norm on \mathbb{R}^p whose unit ball B is given by a polytope. Consider the penalized optimization problem*

$$S_{X,\|\cdot\|}(y) = \text{Arg min}_{b \in \mathbb{R}^p} \frac{1}{2} \|y - Xb\|^2 + \|b\|, \quad (1)$$

where $y \in \mathbb{R}^n$. Let B^* denote the unit ball of the dual norm $\|\cdot\|^*$. There exists $y \in \mathbb{R}^n$ with $|S_{X,\|\cdot\|}(y)| > 1$ if and only if $\text{row}(X)$ intersects a face of the dual unit ball B^* whose codimension is larger than $\text{rk}(X)$.

It should be noted that also vertices are faces (of dimension zero and codimension p), as is the polytope itself (of dimension p and codimension zero), a precise definition for faces is given in the appendix.

As mentioned in the introduction, the notion of uniqueness considered in Theorem 1 is strong in the sense that it guarantees uniqueness for a given design matrix X for all values $y \in \mathbb{R}^n$. This concept of uniqueness is beneficial when studying the stochastic properties of the minimizer in a statistical framework, as then y varies and a criterion independent of y is desirable. Also note that we make no assumptions on X .

If the norm $\|\cdot\|$ involves a tuning parameter λ , the uniqueness of the corresponding penalized problem does not depend on the particular choice of λ . The parameter simply scales B and subsequently B^* and does not affect which faces are intersected by the vector space $\text{row}(X)$.

Theorem 1 generalizes Theorem 14 given in Ewald and Schneider (2020), which provides a necessary and sufficient condition for the uniqueness of the LASSO minimizer: All LASSO solutions are unique if and only if $\text{row}(X)$ only intersects faces of the unit cube $[-1, 1]^p$ whose codimension is less than or equal to $\text{rk}(X)$. Note that the unit cube is, indeed, the corresponding dual to the unit ball of the ℓ_1 -norm.

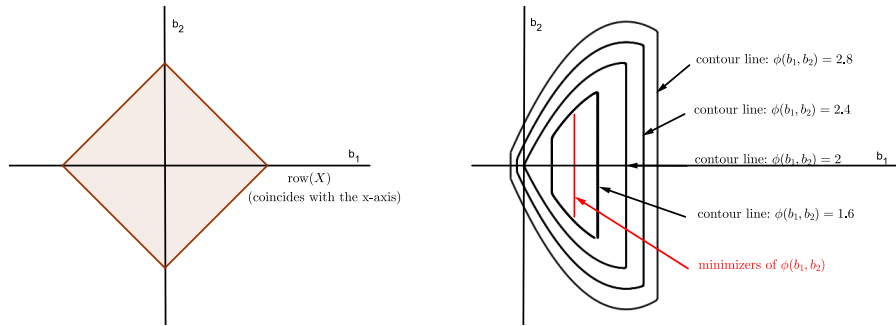
Example 1 *We illustrate the criterion from Theorem 1 for $\|\cdot\| = \|\cdot\|_\infty$, the supremum norm, in Figure 1. Let $X = (1 \ 0)$. The unit dual ball B^* is given by the unit cross-polytope $\text{conv}\{\pm(1,0)', \pm(0,1)'\}$ and we have $\text{rk}(X) = 1$. Clearly, the vertex $(1,0)'$ with codimension $p - 0 = 2 > 1 = \text{rk}(X)$ intersects $\text{row}(X)$, so that one can pick $y \in \mathbb{R}$ for which the set of minimizers $S_{X,\|\cdot\|_\infty}(y)$ is not a singleton. In Figure 1(a), we illustrate this fact for $S_{X,\|\cdot\|_\infty}(2)$.*

Also consider $X = (1 \ 1)$. Because $\text{row}(X)$ does not intersect any vertex of $\text{conv}\{\pm(1,0)', \pm(0,1)'\}$, the solution set $S_{X,\|\cdot\|_\infty}(y)$ is always a singleton. In Figure 1(b), we illustrate this fact for $S_{X,\|\cdot\|_\infty}(2)$.

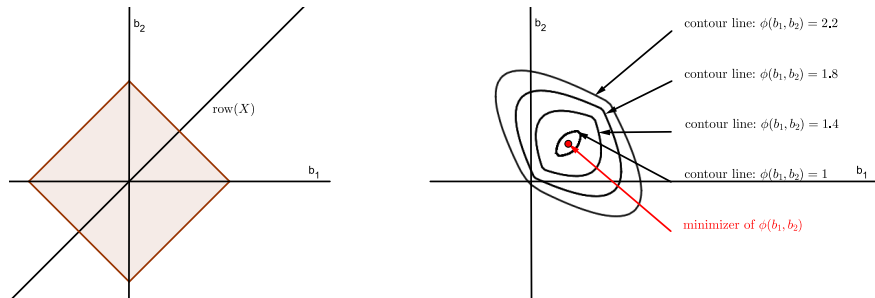
2.1 The related problem of basis pursuit

As mentioned before, the methods of LASSO and basis pursuit (BP) are closely related, as the BP problem can be thought of a LASSO problem with vanishing tuning parameter. More concretely, the setting for BP is the following. Let $X \in \mathbb{R}^{n \times p}$ and let $y \in \text{col}(X)$. The set $S_{X,\text{bp}}(y)$ of BP minimizers is defined as

$$S_{X,\text{bp}}(y) = \text{Arg min } \|b\|_1 \text{ subject to } Xb = y.$$



(a) Let $X = (1 \ 0)$. On the left-hand side, we see that $\text{row}(X)$ intersects a vertex of the cross-polytope whose codimension is 2 and thus is larger than $\text{rk}(X) = 1$. Therefore, there exists $y \in \mathbb{R}$ for which $S_{X, \|\cdot\|_\infty}(y)$ is not a singleton. On the right-hand side, the contour lines of the objective function $\phi(b_1, b_2) = 0.5(2 - b_1)^2 + \max\{|b_1|, |b_2|\}$ show that the set $S_{X, \|\cdot\|_\infty}(2)$ (in red), indeed, contains infinitely many points.



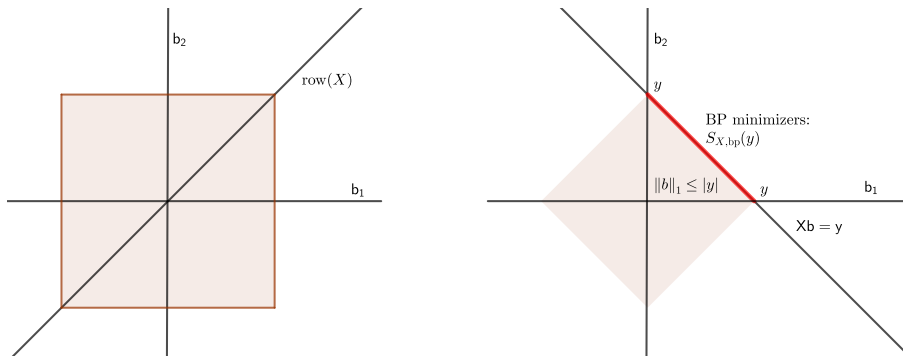
(b) Let $X = (1 \ 1)$. On the left-hand side, we see that $\text{row}(X)$ does not intersect any face of the cross-polytope whose codimension is larger than $\text{rk}(X) = 1$ (such faces are the vertices in this example). Therefore, the set $S_{X, \|\cdot\|_\infty}(y)$ is a singleton for all $y \in \mathbb{R}$. On the right-hand side, the contour lines of the objective function $\phi(b_1, b_2) = 0.5(2 - b_1)^2 + \max\{|b_1|, |b_2|\}$ show that the set $S_{X, \|\cdot\|_\infty}(2)$ (in red) does, indeed, only contain a single point.

Figure 1: Illustration of Theorem 1 for the supremum norm.

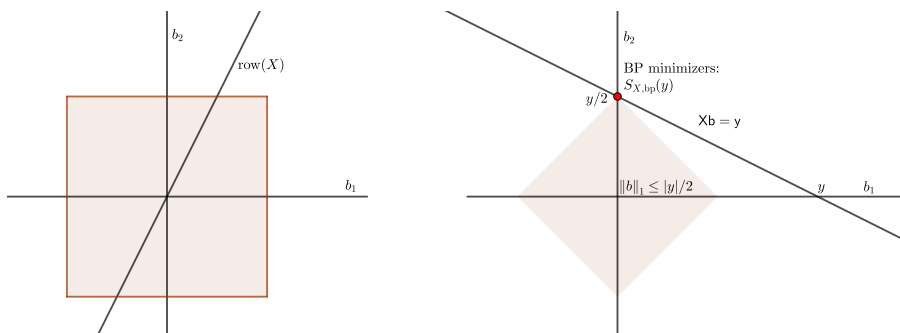
The following theorem shows that, indeed, as BP is a limiting case of the LASSO, the corresponding uniqueness condition – which is independent of the choice of tuning parameter as discussed above – carries over to the BP problem.

Theorem 2 *Let $X \in \mathbb{R}^{n \times p}$. There exists $y \in \text{col}(X)$ for which $|S_{X,\text{bp}}(y)| > 1$ if and only if $\text{row}(X)$ intersects a face of the unit cube $[-1, 1]^p$ whose codimension is larger than $\text{rk}(X)$.*

We illustrate Theorem 2 in Figures 2(a) and 2(b).



(a) Let $X = (1 \ 1)$. On the left-hand side, we see that $\text{row}(X)$ intersects a face of the unit square whose codimension 2 is larger than $\text{rk}(X) = 1$ (which are the vertices in this example). Therefore, by Theorem 2, there exists $y \in \mathbb{R}$ for which the BP minimizer is not unique. The right-hand side illustrates that, indeed, for an arbitrary $y \in \mathbb{R} \setminus \{0\}$, the set $S_{X,\text{bp}}(y)$ (the red segment) is not a singleton.



(b) Let $X = (1 \ 2)$. On the left-hand side, we see that $\text{row}(X)$ does not intersect any face of the unit square whose codimension is larger than $\text{rk}(X) = 1$ (which are the vertices in this example). Therefore, by Theorem 2, the BP minimizer is unique for all $y \in \mathbb{R}$. The right-hand side illustrates that for an arbitrary $y \in \mathbb{R}$, the set $S_{X,\text{bp}}(y)$ (in red) is, indeed, a singleton.

Figure 2: Illustration of Theorem 2.

In the following proposition, we show that the necessary and sufficient condition given in Theorem 1 and therefore also the one given in Theorem 2 is weak. More precisely, we

establish that the set of $X \in \mathbb{R}^{n \times p}$ for which the necessary and sufficient condition given in Theorem 1 does not hold, is negligible with respect to the Lebesgue measure.

Proposition 3 *Let μ be the Lebesgue measure on $\mathbb{R}^{n \times p}$ and let $\|\cdot\|$ be a norm on \mathbb{R}^p whose unit ball is given by a polytope. The following equality holds*

$$\mu(\{X \in \mathbb{R}^{n \times p} : \exists y \in \mathbb{R}^n \text{ with } |S_{X, \|\cdot\|}(y)| > 1\}) = 0.$$

The following corollary is then straightforward given the fact that the LASSO, which is covered by Theorem 1, and BP share the same characterization for uniqueness.

Corollary 4 *Let μ be the Lebesgue measure on $\mathbb{R}^{n \times p}$, then the following equality holds*

$$\mu(\{X \in \mathbb{R}^{n \times p} : \exists y \in \mathbb{R}^n \text{ with } |S_{X, \text{bp}}(y)| > 1\}) = 0.$$

By taking the appropriate norms in Proposition 3, and by Corollary 4, one may deduce that the necessary and sufficient conditions for uniqueness of SLOPE, PACS, fused, clustered and classical LASSO are weak. However, one should be aware that Proposition 3 does not mean that this condition always occurs in practice! For example, for BP (or LASSO), when $p > n$ and $X \in [-1, 1]^{n \times p}$ is a matrix having a row with at least $n + 1$ elements in $\{-1, 1\}$ then, one can pick $y \in \text{col}(X)$ for which the set of minimizers $S_{X, \text{bp}}(y)$ is not a singleton (or, for any $\lambda > 0$, one can pick $y \in \mathbb{R}^n$ for which the set of minimizers $S_{X, \lambda \|\cdot\|_1}(y)$ is not a singleton). Matrices having entries in $\{-1, 1\}$ appear in several theoretical works, such as Rauhut (2010) and Tardivel et al. (2018), and are used for applications in radar and wireless communication (see e.g. Romberg, 2009; Haupt et al., 2010). Moreover, Dupuis and Vaiter (2019) recently illustrated that the matrix $X \in [-1, 1]^{5000 \times 6000}$, having most entries in $\{-1, 1\}$, and the vector $y \in \mathbb{R}^{5000}$ provided by the dataset “gisette” give a set of minimizers $S_{X, \lambda \|\cdot\|_1}(y)$ which is not a singleton once $\lambda > 0$ is small enough.

3. Pattern selection properties

The geometric considerations around Theorems 1 and 2 can also provide insights on the pattern selection aspects of the method under consideration. The keystone is to associate a pattern with a face of the polytope B^* , the unit ball of the dual norm. For LASSO and BP, we exploit the fact that each face of the unit cube corresponds to a sign vector and show that the faces intersected by the row span of X provide the accessible sign vectors for these estimators, see Appendix A. We take a similar, but more sophisticated approach for SLOPE in Section 3.1 where the patterns we consider also carry information about the clustering phenomenon of the method.

In Section 3.2, we take a different angle and characterize the SLOPE null polyhedron and its connection to the sparsity and clustering property of this method. For the LASSO, it is known that the estimation residuals are the projection of y onto the LASSO null polyhedron. We also further generalize this fact to arbitrary norm-penalized least-squares estimation.

3.1 Accessible patterns for SLOPE

We now turn to accessible patterns for SLOPE, whose norm is given by $\|b\|_w = \sum_{j=1}^p w_j |b|_{(j)}$, where $|b|_{(1)} \geq \dots \geq |b|_{(p)}$, as introduced before. For the remainder of Section 3, we assume that the weight vector w of the satisfies

$$w_1 > \dots > w_p > 0,$$

i.e., that all components non-zero and strictly decreasing. (This assumption is not needed for applying Theorem 1 to SLOPE, since $w_1 > 0$ and decreasing components are sufficient for $\|\cdot\|_w$ to be a norm.) We introduce a more sophisticated notion of a ‘‘pattern’’ chosen by SLOPE compared to sign vectors that can account for the clustering property which is not shared by LASSO or BP.

Definition 5 *We say that a vector $m \in \mathbb{Z}^p$ is a SLOPE pattern, if either $m = 0$, or, if for all $l \in [||m||_\infty]$, there exists $j \in [p]$ such that $|m_j| = l$. We denote the set of all SLOPE patterns of dimension p by \mathcal{P}_p . Moreover, for $x \in \mathbb{R}^p$, we define $\text{patt}(x) \in \mathcal{P}_p$ through the following.*

- 1) $\text{sign}(\text{patt}(x)) = \text{sign}(x)$
- 2) $|x_i| = |x_j| \implies |\text{patt}(x)_i| = |\text{patt}(x)_j|$
- 3) $|x_i| > |x_j| \implies |\text{patt}(x)_i| > |\text{patt}(x)_j|$

Example 2 *For $x = (3.1, -1.2, 0, -3.1)'$, we have $\text{patt}(x) = (2, -1, 0, -2)'$. For $x \in \mathbb{R}^4$ with $\text{patt}(x) = (0, 2, 1, -2)'$, we have $\text{sign}(x) = (0, 1, 1, -1)'$ and $|x_2| = |x_4| > |x_3| > x_1 = 0$. The set of all SLOPE patterns in \mathbb{R}^2 is given by*

$$\begin{aligned} \mathcal{P}_2 = \{ & (0, 0)', (1, 0)', (-1, 0)', (0, 1)', (0, -1)', (1, 1)', (1, -1)', (-1, 1)', (-1, -1)', \\ & (2, 1)', (-2, 1)', (2, -1)', (-2, -1)', (1, 2)', (-1, 2)', (1, -2)', (-1, -2)'\}. \end{aligned}$$

The main geometric object of study in this section is the signed permutahedron, which constitutes the dual of the sorted- ℓ_1 -norm unit ball (Proposition 21 in Appendix B.6) and is defined as

$$P_w^\pm = \text{conv} \{ (\sigma_1 w_{\pi(1)}, \dots, \sigma_p w_{\pi(p)})' : \sigma_1, \dots, \sigma_p \in \{-1, 1\}, \pi \in \mathcal{S}_p \}.$$

The shape of this polytope is illustrated in Figure 3 (in two dimensions) and in Figure 4 (in three dimensions). Also of importance will be the permutahedron, defined by

$$P_w = \text{conv} \{ (w_{\pi(1)}, \dots, w_{\pi(p)})' : \pi \in \mathcal{S}_p \}.$$

The permutahedron is, in fact, a face of the signed permutahedron P_w^\pm . We denote the subdifferential of the sorted- ℓ_1 -norm at $x \in \mathbb{R}^p$ by $\partial_{\|\cdot\|_w}(x)$. Any $\partial_{\|\cdot\|_w}(x)$ is a face of P_w^\pm , which we shall denote by $F_w(x)$ in the following.

SLOPE patterns m having only positive components can be interpreted as an ordered partition of $[p]$, where the the smallest and largest element of this partition is the set

$\{j : m_j = 1\}$ and the set $\{j : m_j = \|m\|_\infty\}$, respectively. It is well known that there is a one-to-one relationship between the elements of an ordered partition and the faces of the permutahedron (see e.g. Maes and Kappen, 1992; Simion, 1997; Ziegler, 2012). Instigated by this, we show in Theorem 6 that this result can, indeed, be extended to a one-to-one relationship between all SLOPE patterns and the non-empty faces of the signed permutahedron, which we denote by $\mathcal{F}_0(P_w^\pm)$.

Theorem 6 *The mapping $m \in \mathcal{P}_p \mapsto F_w(m) = \partial_{\|\cdot\|_w}(m)$ is a bijection between the SLOPE patterns \mathcal{P}_p and $\mathcal{F}_0(P_w^\pm)$, the non-empty faces of the signed permutahedron P_w^\pm . In addition, the following holds.*

- 1) *The codimension of $F_w(m)$ is given by $\|m\|_\infty$.*
- 2) *We have $F_w(x) = F_w(\text{patt}(x))$.*

The assumption that components of w are strictly decreasing and non-zero is important. For example, if $w_1 = \dots = w_p > 0$, the signed permutahedron is just a cube and clearly, there is no one-to-one relationship between the set SLOPE patterns and the set of faces of the cube. A similar situation arises if w contains zero components. As can be seen when $p = 2$ and $w_2 = 0$, the sorted- ℓ_1 -norm is the supremum norm and the corresponding dual unit ball is the unit cross-polytope in \mathbb{R}^2 , whose faces cannot bijectively be mapped to \mathcal{P}_2 given in the example above.

Example 3 *We now describe the faces $F_w(m)$, $m \in \mathcal{P}_2$, of the signed permutahedron P_w^\pm when $w = (3.5, 1.5)'$. In the following, we use the fact that – up to an orthogonal transformation described in Lemma 23 – $F_w(m)$ is equal to $F_w(\tilde{m})$ for some \tilde{m} , a non-negative and non-increasing SLOPE pattern. The relationship between the SLOPE patterns $m \in \mathcal{P}_2$ and faces of the signed permutahedron P_w^\pm are listed below and illustrated in Figure 3. Note that $\text{codim}(F_w(m)) = \|m\|_\infty$.*

<i>pattern \tilde{m}</i>	<i>face $F_w(\tilde{m})$</i>	<i>codim.</i>	<i>faces $F_w(m)$ isometric to $F_w(\tilde{m})$</i>
$\tilde{m} = (0, 0)'$	<i>signed permutahedron P_w^\pm</i>	0	–
$\tilde{m} = (1, 0)'$	<i>segment $\{3.5\} \times [-1.5, 1.5]$</i>	1	$m \in \{(-1, 0)', \pm(0, 1)'\}$
$\tilde{m} = (1, 1)'$	<i>permutahedron P_w</i>	1	$m \in \{(-1, -1)', \pm(1, -1)'\}$
$\tilde{m} = (2, 1)'$	<i>point: $(3.5, 1.5)'$</i>	2	$m \in \{(-2, -1)', \pm(2, -1)', \pm(1, 2)', \pm(1, -2)'\}$

Analogously to the accessible sign vectors for LASSO and BP, for a given X , we introduce the notion of accessible SLOPE patterns.

Definition 7 (Accessible SLOPE pattern) *Let $X \in \mathbb{R}^{n \times p}$ and $m \in \mathcal{P}_p$. We say that m is an accessible SLOPE pattern with respect to X if*

$$\exists y \in \mathbb{R}^n \text{ and } \exists \hat{\beta} \in S_{X, \|\cdot\|_w}(y) \text{ such that } \text{patt}(\hat{\beta}) = m.$$

We now provide a geometric and analytic characterization of accessible SLOPE patterns.

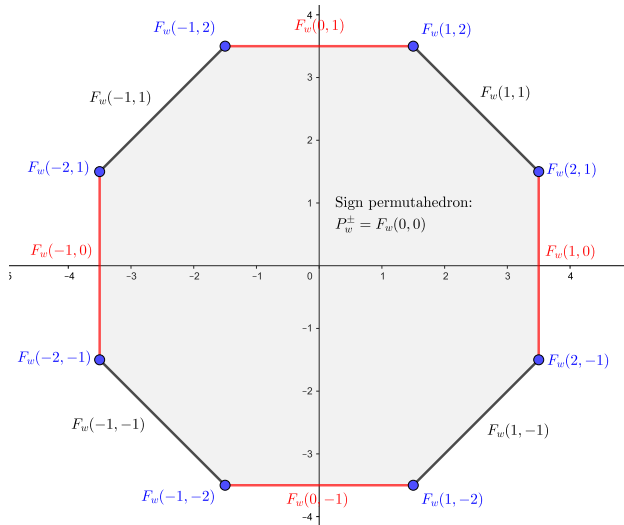


Figure 3: Illustration of the relationship between the SLOPE patterns and the faces of the signed permutahedron P_w^\pm for $w = (3.5, 1.5)'$ through subdifferential calculus, see Proposition 16 in Appendix B.3 and Proposition 21 in Appendix B.6. Note that $F_w(m) = \partial_{\|\cdot\|_w}(m)$. Faces having the same color are isometric. One may notice that $\text{codim}(F_w(m)) = \|m\|_\infty$.

Theorem 8 (Characterization of accessible SLOPE patterns) *Let $X \in \mathbb{R}^{n \times p}$.*

- 1) *Geometric characterization: A SLOPE pattern $m \in \mathcal{P}_p$ is accessible with respect to X if and only if $\text{row}(X)$ intersects the face $F_w(m)$.*
- 2) *Analytic characterization: A SLOPE pattern $m \in \mathcal{P}_p$ is accessible with respect to X if and only if the implication*

$$Xb = Xm \implies \|b\|_w \geq \|m\|_w$$

holds.

We point out that the analytic characterization allows to check accessibility of a particular SLOPE pattern by in fact minimizing a BP-like problem where the ℓ_1 -norm is replaced by the sorted- ℓ_1 -norm. This in turn can give insight on whether the corresponding face of the signed permutahedron is intersected by $\text{row}(X)$.

Also note that the set of accessible SLOPE patterns is invariant by scaling w with a constant, since $\text{row}(X)$ intersects $F_w(m)$ if and only if $\text{row}(X)$ intersects $F_{\lambda w}(m)$ with $\lambda > 0$. The following corollary, which is in line with Theorem 2.1 very recently given in Kremer et al. (2022), is a straightforward consequence of Theorems 1, 6 and 8.

Corollary 9 *Let $X \in \mathbb{R}^{n \times p}$. If $\text{row}(X)$ does not intersect any face of P_w^\pm with codimension larger than $\text{rk}(X)$, then for all $y \in \mathbb{R}^n$, $\hat{\beta}_w(y)$, the unique element of $S_{X, \|\cdot\|_w}(y)$, satisfies $\|\text{patt}(\hat{\beta}_w(y))\|_\infty \leq \text{rk}(X)$.*

Corollary 9 generalizes the well-known fact that, when uniqueness occurs, the LASSO minimizer has less than $\text{rk}(X)$ non-null components. Indeed, the above corollary shows that when the SLOPE minimizer is unique, the number of non-null clusters is less than or equal to $\text{rk}(X)$.

Example 4 We illustrate the criterion for accessible SLOPE patterns from Theorem 8 for $w = (5.5, 3.5, 1.5)'$ and X given by

$$X = \begin{pmatrix} 8 & 5 & 8 \\ 10 & 1.25 & -6 \end{pmatrix}.$$

Table 1 lists all accessible non-null SLOPE patterns ($m = 0$ is always accessible through $y = 0$), the geometric illustration is shown in Figure 4.

colour	type	intersection $\neq \emptyset$	face intersected isom. to	SLOPE patt.
orange	segments	$\text{row}(X) \cap F_w(\pm(1, 0, 0))$	$\{5.5\} \times P_{(3.5, 1.5)}^\pm$	$\pm(1, 0, 0)$
red	segments	$\text{row}(X) \cap F_w(\pm(1, 1, 1))$	$P_{(5.5, 3.5, 1.5)}$	$\pm(1, 1, 1)$
black	segments	$\text{row}(X) \cap F_w(\pm(0, 0, 1))$	$\{5.5\} \times P_{(3.5, 1.5)}^\pm$	$\pm(0, 0, 1)$
pink	segments	$\text{row}(X) \cap F_w(\pm(-1, 0, 1))$	$P_{(5.5, 3.5)} \times [-1.5, 1.5]$	$\pm(-1, 0, 1)$
purple	points	$\text{row}(X) \cap F_w(\pm(2, 0, -1))$	$\{5.5\} \times \{3.5\} \times [-1.5, 1.5]$	$\pm(2, 0, -1)$
green	points	$\text{row}(X) \cap F_w(\pm(2, 1, 1))$	$\{5.5\} \times P_{(3.5, 1.5)}$	$\pm(2, 1, 1)$
blue	points	$\text{row}(X) \cap F_w(\pm(1, 1, 2))$	$\{5.5\} \times P_{(3.5, 1.5)}$	$\pm(1, 1, 2)$
yellow	points	$\text{row}(X) \cap F_w(\pm(-1, 0, 2))$	$\{5.5\} \times \{3.5\} \times [-1.5, 1.5]$	$\pm(-1, 0, 2)$

Table 1: Accessible SLOPE patterns with respect to $X = \begin{pmatrix} 8 & 5 & 8 \\ 10 & 1.25 & -6 \end{pmatrix}$ and $w = (5.5, 3.5, 1.5)'$.

3.2 The SLOPE null polyhedron and a general result

In the previous section, we gave a description of accessible SLOPE patterns based on the intersection of $\text{row}(X)$ with the signed permutahedron P_w^\pm . In this section, our aim is the following: Given an accessible pattern $m \in \mathcal{P}_p$, we want to provide the set of $y \in \mathbb{R}^n$ for which there exists $\hat{\beta} \in S_{X, \|\cdot\|_w}(y)$ with $\text{patt}(\hat{\beta}) = m$. In other words, we want to describe the set

$$A_w(m) = \{y \in \mathbb{R}^n : \exists \hat{\beta} \in S_{X, \|\cdot\|_w}(y) \text{ where } \text{patt}(\hat{\beta}) = m\}.$$

Note that when the SLOPE minimizer is unique, the sets $A_w(m)$ and $A_w(\tilde{m})$ are disjoint for $m \neq \tilde{m}$, whereas $A_w(m) \cap A_w(\tilde{m}) \neq \emptyset$ might occur in case of non-uniqueness. Clearly, the null pattern $m = 0$ is accessible. The corresponding set $A_w(0)$, called the *SLOPE null polyhedron*, given by

$$A_w(0) = \{y \in \mathbb{R}^n : \|X'y\|_w^* \leq 1\}$$

by Proposition 18. This is the set of all y such that $X'y \in P_w^\pm$, which is again a polytope. The proposition below shows that the faces of this polytope $N_w(m) = \{f \in \mathbb{R}^n : X'f \in F_w(m)\}$ for the *accessible* SLOPE patterns m are the cornerstone to describe the sets $A_w(m)$.

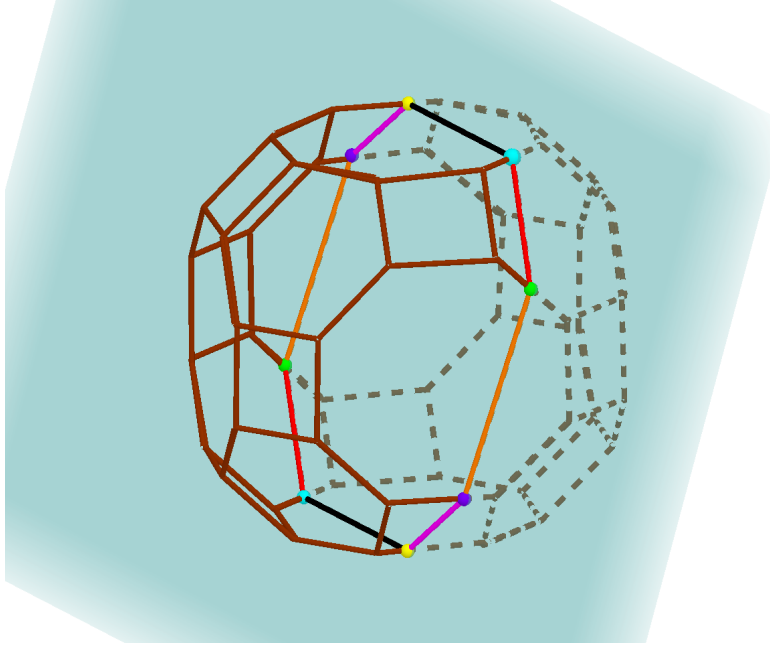


Figure 4: Illustration of the signed permutahedron P_w^\pm (in brown) and the plane $\text{row}(X)$ (in light blue). Because $\text{rk}(X) = 2$ and $\text{row}(X)$ does not intersect any vertex of P_w^\pm (the faces with codimension equal to 3), the SLOPE estimator $\hat{\beta}_w(y)$ is unique for all values of $y \in \mathbb{R}^2$. Colored segments and points are the intersections between $\text{row}(X)$ and the faces of P_w^\pm , determining the accessible SLOPE patterns shown in Table 1. For example, $m = (2, 1, 1)'$ is an accessible SLOPE pattern, which implies that there exists $y \in \mathbb{R}^2$ for which the SLOPE minimizer $\hat{\beta}_w(y)$ satisfies $\hat{\beta}_w(y)_1 > \hat{\beta}_w(y)_2 = \hat{\beta}_w(y)_3 > 0$. In addition, since $m = (2, 1, 0)'$ is not an accessible pattern, one cannot pick $y \in \mathbb{R}^2$ for which the SLOPE minimizer satisfies $\hat{\beta}_w(y)_1 > \hat{\beta}_w(y)_2 > \hat{\beta}_w(y)_3 = 0$.

Proposition 10 *Let $X \in \mathbb{R}^{n \times p}$. The SLOPE pattern $m \in \mathcal{P}_p$ is an accessible SLOPE pattern if and only if $N_w(m) = \{f \in \mathbb{R}^n : X'f \in F_w(m)\} \neq \emptyset$. In that case, the set $A_w(m)$ is given by*

$$A_w(m) = \{y = f + Xb : f \in N_w(m), \text{patt}(b) = m\}.$$

Note that Proposition 10 yields another characterization of accessible SLOPE patterns, namely that m is accessible if and only if $N_w(m)$ is a non-empty face of the SLOPE null polyhedron. In case of non-uniqueness, different patterns may yield the same face, so one should be aware that there is no bijection between the accessible SLOPE patterns and the faces of the SLOPE null polytope. Also note that if $\text{rk}(X) = n$ and we are given the intersection between $\text{row}(X)$ and $F_w(m)$ for some accessible SLOPE pattern m , we can write $N_w(m) = (XX')^{-1}X(\text{row}(X) \cap F_w(m))$ since

$$f \in N_w(m) \iff X'f \in \text{row}(X) \cap F_w(m) \iff f \in (XX')^{-1}X(\text{row}(X) \cap F_w(m)).$$

Example 5 *Figure 4 illustrates the accessible SLOPE patterns from Theorem 8 for $w = (5.5, 3.5, 1.5)'$ and*

$$X = \begin{pmatrix} 8 & 5 & 8 \\ 10 & 1.25 & -6 \end{pmatrix}.$$

Now, for every accessible SLOPE pattern, Figure 5 below provides the set $A_m = \{y \in \mathbb{R}^2 : \exists \hat{\beta} \in S_{X, \|\cdot\|_w}(y) \text{ where } \text{patt}(\hat{\beta}) = m\}$ and the SLOPE null polyhedron.

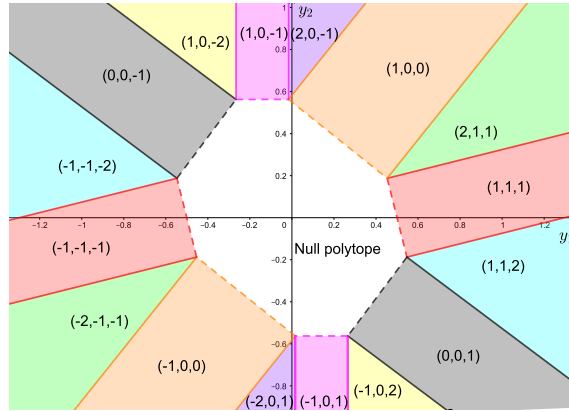


Figure 5: Illustration of the SLOPE null polytope and the accessible patterns for $X = \begin{pmatrix} 8 & 5 & 8 \\ 10 & 1.25 & -6 \end{pmatrix}$ and $w = (5.5, 3.5, 1.5)'$. The resulting accessible patterns are $\{\pm(1, 0, 0), \pm(1, 1, 1), \pm(0, 0, 1), \pm(-1, 0, 1), \pm(2, 0, -1), \pm(2, 1, 1), \pm(1, 1, 2), \pm(-1, 0, 2)\}$, each associated with a face of the polytope. Depicted also are the sets $A_w(m) = \{y \in \mathbb{R}^2 : \exists \hat{\beta} \in S_{X, \|\cdot\|_w}(y) \text{ with } \text{patt}(\hat{\beta}) = m\}$ for each accessible pattern.

Note that the SLOPE null polyhedron $A_w(0)$ can also be interpreted as the set of SLOPE residuals in the sense that $\hat{u} = y - X\hat{\beta}$ is the projection of y onto $A_w(0)$ whenever $\hat{\beta} \in S_{X, \|\cdot\|_w}(y)$ (Minami, 2020). Or put differently again, we can decompose y as $y = X\hat{\beta} + \hat{u}$, where $X\hat{\beta}$ is the SLOPE fit and $\hat{u} \in A_w(0)$, the set of all values that lead to a zero SLOPE

minimizer. This property is well known also for the LASSO, (c.f. Tibshirani and Taylor, 2012). In fact, it is straightforward to see from Proposition 18 that the same considerations hold for all problems as defined in (1). For completeness, we summarize this in the following proposition which holds for arbitrary norms.

Proposition 11 *Let $X \in \mathbb{R}^{n \times p}$ and $y \in \mathbb{R}^n$ and let $\|\cdot\|$ be a norm on \mathbb{R}^p . Define the convex null set $A_\emptyset = \{u \in \mathbb{R}^n : \|X'u\|^* \leq 1\}$. We then have $S_{X,\|\cdot\|}(u) = \{0\}$ for all $u \in A_\emptyset$, and any $\hat{\beta} \in S_{X,\|\cdot\|}(y)$ satisfies $y = X\hat{\beta} + \hat{u}$ with $\hat{u} \in A_\emptyset$. Moreover, \hat{u} is the projection of y onto A_\emptyset .*

4. Conclusion and perspective

In Theorem 1, we provide a necessary and sufficient condition for the uniqueness of penalized least-squares estimators whose penalty term is given by a norm with a polytope-shaped unit ball. To the best of our knowledge, this kind of uniqueness has not been treated in this generality before, only a necessary and sufficient condition in the special case of the LASSO has been available. Our condition involves a new geometric approach that allows to also investigate other properties of these types of methods. A central role in this approach is played by the unit ball of the norm that is dual to the penalizing term, denoted by B^* . For the LASSO, it is fairly straightforward to see that every possible signed model corresponds to a face of B^* , the unit cube in this case. For SLOPE, we show that B^* is, in fact, given by the so-called signed permutahedron. We also show the highly non-trivial fact that there is a one-to-one correspondence between the faces of this signed permutahedron and the so-called SLOPE patterns, which contain the information about zero components, signs, clusters, and the ordering in a SLOPE solution. Our findings illustrate the intrinsic connection between the faces of the geometric object B^* and the type of patterns the corresponding penalized method can uncover. This suggests to further explore this link generally in penalized estimation, which could, for example, be accomplished by the implicit definition that patterns are equivalence classes of elements sharing the same subdifferential with respect to the penalty term. Another natural direction for extending the uniqueness result (and also the results for pattern selection) would be to consider even more general penalties to also encompass methods such as the generalized LASSO and related procedures which are currently not covered in our setting.

5. Acknowledgments

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Appendix A. Appendix – Accessible sign vectors for LASSO and BP

We start by introducing the notion of accessible sign vectors for LASSO and BP problems.

Definition 12 (Accessible sign vectors for LASSO and BP) *Let $X \in \mathbb{R}^{n \times p}$, $\sigma \in \{-1, 0, 1\}^p$, and $\lambda > 0$. We say that σ is an accessible sign vector for LASSO (or BP) with respect to X , if there exists $y \in \mathbb{R}^n$ and $\hat{\beta} \in S_{X, \lambda, \|\cdot\|_1}(y)$ (or there exists $y \in \text{col}(X)$ and $\hat{\beta} \in S_{X, \text{bp}}(y)$, respectively), such that $\text{sign}(\hat{\beta}) = \sigma$.*

The following theorem provides a geometric characterization of accessible sign vectors for LASSO and BP based on faces of the unit cube $[-1, 1]^p$ and the vector space $\text{row}(X)$. First, note that sub-differential calculus of the ℓ_1 -norm at $\sigma \in \{-1, 0, 1\}^p$ gives

$$\partial_{\|\cdot\|_1}(\sigma) = E_1 \times \cdots \times E_p \text{ with } E_j = \begin{cases} \{\sigma_j\} & |\sigma_j| = 1 \\ [-1, 1] & \sigma_j = 0, \end{cases}$$

where $\partial_{\|\cdot\|_1}(x)$ denotes the subdifferential of the ℓ_1 -norm at $x \in \mathbb{R}^p$, see Appendices B.1 and B.3 for more details. Therefore, the mapping $\sigma \mapsto \partial_{\|\cdot\|_1}(\sigma)$ is a bijection between sign vectors in $\{-1, 0, 1\}^p$ and faces of the unit cube in \mathbb{R}^p . We let $F_1(\sigma) = \partial_{\|\cdot\|_1}(\sigma)$ in the following. For completeness, Theorem 13 also contains an analytic characterization of accessibility.

Theorem 13 (Characterization of accessible LASSO and BP sign vectors) *Let $X \in \mathbb{R}^{n \times p}$ and $\lambda > 0$.*

- 1) *Geometric characterization: A sign vector $\sigma \in \{-1, 0, 1\}^p$ is accessible for LASSO or BP with respect to X if and only if $\text{row}(X)$ intersects the face $F_1(\sigma)$.*
- 2) *Analytic characterization: A sign vector $\sigma \in \{-1, 0, 1\}^p$ is accessible for LASSO or BP with respect to X if and only if the implication*

$$Xb = X\sigma \implies \|b\|_1 \geq \|\sigma\|_1$$

holds.

The analytic characterization for accessible sign vectors is, in fact, closely related to the identifiability condition given in Tardivel and Bogdan (2022), in which the inequality above is replaced by a strict inequality. In high-dimensional linear regression, this condition is necessary and sufficient for sign recovery of thresholded LASSO and thresholded BP (Tardivel and Bogdan, 2022), as well as for so-called thresholded justice pursuit (Descloux et al., 2022), a method closely related to BP. We point out that the analytic characterization allows to check accessibility of a particular sign vector simply by solving a BP problem, which in turn gives insight on whether the corresponding face of the unit cube is intersected by $\text{row}(X)$. In practice, one does not even need an accurate numerical solver to check whether a sign vector $\sigma \in \{-1, 0, 1\}^p$ is accessible, when the BP problem is uniquely solvable: if we are given an approximate minimizer $\tilde{\beta}$ for the BP problem with $y = X\sigma$ that satisfies $\|\tilde{\beta} - \hat{\beta}\|_\infty < 1/2$, where $\hat{\beta}$ is the exact minimizer, it suffices to check whether

$\text{sign}(\text{round}(\tilde{\beta})) = \sigma$, where $\text{round}(\cdot)$ rounds componentwise to the closest integer. In that case, σ is accessible, whereas σ is not accessible if $\text{sign}(\text{round}(\tilde{\beta})) \neq \sigma$, as outlined in Corollary 26 in Appendix B.10. This approach to check accessibility was used in Tardivel and Bogdan (2022) to derive the so-called identifiability curve.

Note that Theorem 13 reveals that whether a sign vector is accessible for LASSO does not depend on the value of the tuning parameter λ . We also point out that Theorems 1 and 13 allow to deduce that the number of non-null components of the LASSO is always less than or equal to $\text{rk}(X)$ when the solutions are unique. Indeed, if the LASSO minimizer is unique, according to Theorem 1, $\text{row}(X)$ does not intersect a face of $[-1, 1]^p$ associated to a sign vector having more than $\text{rk}(X)$ non-null components, i.e., a face whose codimension is larger than $\text{rk}(X)$. This implies that only sign vectors with at most $\text{rk}(X)$ components different to zero are accessible. For the LASSO, this is a refined version of the well-known fact that, in case the estimator is unique, at most n components can be non-zero (see e.g. Tibshirani, 2013; Osborne et al., 2000).

Appendix B. Appendix – Proofs

In the appendix, we additionally make use of the following notation. Let A be a matrix. We use the symbol A_j to denote the j -th column of A . For an index set I , A_I is the matrix containing columns with indices in I only. For a vector x , $\text{supp}(x)$ contains the indices of the non-zero components of x . The symbol $|x|_{(j)}$ denotes the j -th order statistic of the absolute values of the components of x , i.e., $|x|_{(1)} \geq |x|_{(2)} \geq \dots$. Let $l, k \in \mathbb{N}$ with $l \leq k$, then $[l : k]$ denotes the set $\{l, l+1, \dots, k\}$. We let $\mathbf{1}_m$ stand for the vector $(1, \dots, 1)' \in \mathbb{R}^m$. All inequalities involving vectors are understood componentwise.

B.1 Facts about subdifferentials

We remind the reader of some definitions and facts on subgradients and subdifferentials. The following can, for instance, be found in Hiriart-Urruty and Lemarechal (1993). For a function $f : \mathbb{R}^p \rightarrow \mathbb{R}$, a vector $s \in \mathbb{R}^p$ is a *subgradient of f at $x \in \mathbb{R}^p$* if

$$f(z) \geq f(x) + s'(z - x) \quad \forall z \in \mathbb{R}^p. \quad (2)$$

The set of all subgradients of f at x , which is a convex set, is called the *subdifferential of f at x* , denoted by $\partial_f(x)$. It is straightforward to characterize the minimizer of a function in the following way

$$x^* \in \text{Arg min } f \iff 0 \in \partial_f(x^*). \quad (3)$$

While convexity of f is not necessary for the above statement, the use of subdifferentials is an especially important tool when this is the case. Given that f is convex, subdifferentiability is also a local property in the sense that for any $\delta > 0$, we have

$$s \in \partial_f(x) \iff f(x+h) \geq f(x) + s'h \text{ for all } h : \|h\|_\infty \leq \delta. \quad (4)$$

B.2 Facts about polytopes

We report some basic definitions and facts on polytopes, which we will use throughout the article and, in particular, in the proofs in subsequent sections. The following can, for instance, be found in the excellent textbooks by Gruber (2007) and Ziegler (2012).

A set $P_{\mathcal{V}} \subseteq \mathbb{R}^p$ is called a \mathcal{V} -polytope, if it is the convex hull of a finite set of points in \mathbb{R}^p , namely,

$$P_{\mathcal{V}} = \text{conv}(V_1, \dots, V_k) = \text{conv}(V)$$

for $V = (V_1 \dots V_k) \in \mathbb{R}^{p \times k}$. A set $P_{\mathcal{H}} \subseteq \mathbb{R}^p$ is called an \mathcal{H} -polyhedron, if it is the intersection of a finite number of half-spaces, namely,

$$P_{\mathcal{H}} = \bigcap_{l=1}^m \{x \in \mathbb{R}^p : A'_l x \leq b_l\} = \{x \in \mathbb{R}^p : A'x \leq b\},$$

for some $A = (A_1 \dots A_m) \in \mathbb{R}^{p \times m}$ and $b \in \mathbb{R}^m$. A bounded \mathcal{H} -polyhedron is called \mathcal{H} -polytope. A set $P \subseteq \mathbb{R}^p$ is an \mathcal{H} -polytope if and only if it is a \mathcal{V} -polytope. We therefore simply use the term *polytope* in the following. The *dimension* $\dim(P)$ of a polytope is given by the dimension of $\text{aff}(P)$, the affine subspace spanned by P , and its codimension by $\text{codim}(P) = p - \dim(P)$. A *face* F of P is any subset $F \subseteq P$ that satisfies

$$F = \{x \in P : a'x = b_0\}, \text{ where } P \subseteq \{x : a'x \leq b_0\},$$

for some $a \in \mathbb{R}^p$ and $b_0 \in \mathbb{R}$. Such an inequality $a'x \leq b_0$ is called a *valid inequality* of P . Note that $F = \emptyset$ and $F = P$ are faces of P and that any face F is again a polytope. A face $F \neq P$ is called *proper*. A face of dimension 0 is called *vertex*, and we denote the set of all vertices of P by $\text{vert}(P)$. This set satisfies $\text{vert}(P) \subseteq \{V_1, \dots, V_k\}$, where $P = \text{conv}(V_1, \dots, V_k)$. A point $x_0 \in P$ lies in $\text{relint}(P)$, the *relative interior* of P , if x_0 is not contained in a proper face of P . Finally, the (*polar*) *dual* of P is defined as

$$P^* = \{s \in \mathbb{R}^p : s'x \leq 1 \forall x \in P\},$$

which is again a polytope. We now list a number of useful facts about polytopes involving the above definitions, which are used throughout the article. These properties can either be found explicitly or as a straightforward consequence of properties listed in the above mentioned references.

Proposition 14 *Let $P \in \mathbb{R}^p$ be a polytope given by $P = \text{conv}(V)$, where $V = (V_1, \dots, V_k) \in \mathbb{R}^{p \times k}$, and denote by P^* the dual of P . For simplicity, we assume that $\text{vert}(P) = \{V_1, \dots, V_k\}$. Moreover, let $0 \in P$. The following properties hold.*

- 1) *If F and \tilde{F} are faces of P , then so is $F \cap \tilde{F}$.*
- 2) *For any face F of P , $F = \text{conv}(\text{vert}(P) \cap F)$.*
- 3) *Let D be an affine line contained in the affine span of P . If $D \cap \text{relint}(P) \neq \emptyset$ then D intersects a proper face of P .*
- 4) *We can write $P^* = \{s \in \mathbb{R}^p : V's \leq \mathbf{1}_k\}$.*
- 5) *Any face F^* of P^* can be written as $F^* = \{s \in P^* : V'_I s = \mathbf{1}_{|I|}\}$ for some $I \subseteq [k]$.*
- 6) *Let $I \subseteq [k]$. $F = \text{conv}(V_I)$ is a face of $P \iff F^* = \{s \in P^* : V'_I s = \mathbf{1}_{|I|}\}$ is a face of P^* , where I is the maximal index set in this representation.*
In this case, F^ is the dual of F (and vice versa), and $\text{codim}(F^*) = \text{rk}(V_I)$.*

B.3 Facts about subdifferentials of norms with polytope unit balls

We now consider subdifferentials of norms and list several properties in the following. In particular, we show in Proposition 15 that the subdifferential of a norm evaluated at zero is simply given by the unit ball of the corresponding dual norm, a fact that will be used throughout subsequent proofs. Proposition 16 then shows that all faces of this dual norm unit ball can be represented by a subdifferential of the original norm, provided that this norm is such that its unit ball, and therefore also the unit ball of its dual norm, are given by a polytope. Lemma 17 contains a technical result needed for the proof of Theorem 1.

A version of the following proposition – which holds independently of the shape of the unit ball of the norm under consideration – can also be found in Hiriart-Urruty and Lemarechal (1993).

Proposition 15 *Let $\|\cdot\|$ be a norm on \mathbb{R}^p , and let $\|\cdot\|^*$ denote the dual norm. Then the following holds.*

1) *The subdifferential of $\|\cdot\|$ at 0 is given by*

$$\partial_{\|\cdot\|}(0) = \{s \in \mathbb{R}^p : \|s\|^* \leq 1\}.$$

2) *In general, the subdifferential of $\|\cdot\|$ at x is given by*

$$\partial_{\|\cdot\|}(x) = \{s \in \mathbb{R}^p : \|s\|^* \leq 1, s'x = \|x\|\}.$$

Proof

It suffices to show 2). By definition, we have

$$\partial_{\|\cdot\|}(x) = \{s \in \mathbb{R}^p : \|v\| \geq \|x\| + s'(v - x) \forall v \in \mathbb{R}^p\}$$

Take $s \in \partial_{\|\cdot\|}(x)$. When $v = 0$, we get $s'x \geq \|x\|$. When $v = 2x$, we may deduce that $s'x \leq \|x\|$, implying that $s'x = \|x\|$ must hold. This also implies $\|v\| \geq s'v$ for all $v \in \mathbb{R}^p$, so that $s \in B^*$, yielding

$$\partial_{\|\cdot\|}(x) \subseteq \{s \in B^* : s'x = \|x\|\}.$$

To see that also the converse is true, take any $s \in B^*$ satisfying $s'x = \|x\|$. Now, take any $v \in \mathbb{R}^p$. Clearly $\|v\| \geq s'v = \|x\| + s'(v - x)$, implying that

$$\{s \in B^* : s'x = \|x\|\} \subseteq \partial_{\|\cdot\|}(x).$$

■

Proposition 16 *Let $\|\cdot\|$ be a norm whose unit ball B is the polytope $\text{conv}(V)$ for some $V = (V_1 \dots V_k) \in \mathbb{R}^{p \times k}$. Let $F \subseteq B^*$, where B^* is the dual norm unit ball, with $F \neq \emptyset$. Then*

$$F \text{ is a face of } B^* \iff F = \partial_{\|\cdot\|}(x) \text{ for some } x \in \mathbb{R}^p.$$

Proof (\implies) If $F = B^*$, then $x = 0$ by Proposition 15. If F is a proper face, we can write $F = \{s \in B^* : V'_I s = \mathbf{1}_{|I|}\}$ for some $I \subseteq [k]$, where I is the maximal set satisfying this. Let $x = \sum_{l \in I} V_l$. Since $x/|I| \in \text{conv}(V_I)$, a proper and non-empty face of B , we have $\|x\| = |I|$. Note that for $s \in B^*$, we have $s'V_l \leq 1$, so that

$$s \in \partial_{\|\cdot\|}(x) \iff s'x = \sum_{l \in I} V'_l s = \|x\| = |I| \iff V'_l s = 1 \quad \forall l \in I \iff s \in F.$$

(\impliedby) If $F = \partial_{\|\cdot\|}(x)$, then $F = \{s \in B^* : s'x = \|x\|\}$ by Proposition 15. Since $(x/\|x\|)'s \leq 1$ clearly is a valid inequality for all $s \in B^*$, F is a face of B^* . \blacksquare

Lemma 17 *Let $\|\cdot\|$ be a norm whose unit ball B is the polytope $\text{conv}(V)$ for some $V = (V_1 \dots V_k) \in \mathbb{R}^{p \times k}$. Let $F = \{s \in B^* : V'_I s = \mathbf{1}_{|I|}\}$ be a face of B^* , the dual norm unit ball, and let I be the maximal set satisfying this. Then the following holds.*

$$F \subseteq \partial_{\|\cdot\|}(b) \implies b \in \text{col}(V_I).$$

Proof Since $b/\|b\| \in B = \text{conv}(V)$, we can write $b = \sum_{l=1}^k \alpha_l V_l$ with $\alpha_l \geq 0$ and $\sum_{l=1}^k \alpha_l = \|b\|$. Since $\partial_{\|\cdot\|}(b) = \{s \in B^* : s'b = \|b\|\}$ and $s'V_l \leq 1$, we have for $A = \text{supp}(\alpha)$ and any $s \in \partial_{\|\cdot\|}(b)$

$$\|b\| = s'b = \sum_{l \in A} \alpha_l s'V_l \leq \sum_{l \in A} \alpha_l = \|b\|.$$

This implies that $s'V_l = 1$ for all $l \in \text{supp}(\alpha)$, which, since $F \subseteq \partial_{\|\cdot\|}(b)$, yields $\text{supp}(\alpha) \subseteq I$. \blacksquare

B.4 Proofs of Theorems 1 and 2

The proofs of Theorems 1 and 2 follow a similar outline, with the proof of Theorem 2 being more accessible. We therefore start with the latter one.

B.4.1 CHARACTERIZATION OF BP MINIMIZERS AND PROOF OF THEOREM 2

The following characterization of BP minimizers will prove useful in the following. It can be found in Zhang et al. (2015) and Gilbert (2017), as well as in general form in Mousavi and Shen (2019).

Let $y \in \text{col}(X)$ and let $\hat{\beta}$ satisfy $X\hat{\beta} = y$ then, $\hat{\beta} \in S_{X,\text{bp}}(y)$ if and only if

$$\exists z \in \mathbb{R}^n \text{ such that } \begin{cases} \|X'z\|_\infty \leq 1, \\ X'_j z = \text{sign}(\hat{\beta}_j) \quad \forall j \in \text{supp}(\hat{\beta}). \end{cases} \quad (5)$$

Proof [Proof of Theorem 2]

(\impliedby) Let us assume that $\text{row}(X)$ intersects a face F of $[-1, 1]^p$ whose codimension is larger than $\text{rk}(X)$. We show that one can find some $y \in \text{col}(X)$ for which $S_{X,\text{bp}}(y)$ is not a singleton.

The face F can be written as $F = E_1 \times \cdots \times E_p$, where $E_j \in \{\{-1\}, \{1\}, [-1, 1]\}$ for $j \in [p]$. Now, let $J = \{j \in [p] : |E_j| = 1\}$, the set of indices of sets E_j that are singletons. We have $\text{codim}(F) = |J|$ and, by assumption, $|J| > \text{rk}(X)$. Now define $\hat{\beta} \in \mathbb{R}^p$ by setting

$$\hat{\beta}_j = \begin{cases} 1 & E_j = \{1\} \\ -1 & E_j = \{-1\} \\ 0 & j \notin J. \end{cases}$$

Clearly, $\text{supp}(\hat{\beta}) = J$. Set $y = X\hat{\beta}$. Since $\text{row}(X)$ intersects F , there exists $z \in \mathbb{R}^n$ such that $X'z \in F$. This implies that $\|X'z\|_\infty \leq 1$ and $X'_j z = \hat{\beta}_j = \text{sign}(\hat{\beta}_j)$ for any $j \in \text{supp}(\hat{\beta}) = J$. Therefore, by (5), $\hat{\beta} \in S_{X, \text{bp}}(y)$.

To show that $\hat{\beta}$ is not a unique minimizer, we provide $\tilde{\beta} \in \mathbb{R}^p$ with $\tilde{\beta} \neq \hat{\beta}$, $X\tilde{\beta} = y$ and $\|\tilde{\beta}\|_1 = \|\hat{\beta}\|_1$. Since $|J| > \text{rk}(X)$, the columns of X_J are linearly dependent, so that we can pick $h \in \ker(X)$, $h \neq 0$ such that $\text{supp}(h) \subseteq J$ and $\|h\|_\infty < 1$. Since $\|h\|_\infty < 1$, $\text{sign}(\hat{\beta} + h) = \text{sign}(\hat{\beta}) = \hat{\beta}$. Let $\tilde{\beta} = \hat{\beta} + h$. Note that $X\tilde{\beta} = X\hat{\beta} = y$ and that

$$\begin{aligned} \|\tilde{\beta}\|_1 &= \sum_{j=1}^p \text{sign}(\hat{\beta}_j + h_j)(\hat{\beta}_j + h_j) = \sum_{j=1}^p \text{sign}(\hat{\beta}_j)\hat{\beta}_j + \sum_{j \in J} \hat{\beta}_j h_j = \|\hat{\beta}\|_1 + \sum_{j \in J} (X'z)_j h_j \\ &= \|\hat{\beta}\|_1 + z'Xh = \|\hat{\beta}\|_1, \end{aligned}$$

implying that $\tilde{\beta} \in S_{X, \text{bp}}(y)$ also.

(\implies) We assume that $\hat{\beta}, \tilde{\beta} \in S_{X, \text{bp}}(y)$ with $\hat{\beta} \neq \tilde{\beta}$ for some $y \in \text{col}(X)$. We need to show that there exists a face F of $[-1, 1]^p$ with $F \cap \text{row}(X) \neq \emptyset$ and $\text{codim}(F) > \text{rk}(X)$. Consider $F = E_1 \times \cdots \times E_p$ and $\tilde{F} = \tilde{E}_1 \times \cdots \times \tilde{E}_p$ with

$$E_j = \begin{cases} \{\text{sign}(\hat{\beta}_j)\} & \text{if } j \in \text{supp}(\hat{\beta}) \\ [-1, 1] & \text{if } j \notin \text{supp}(\hat{\beta}) \end{cases} \quad \text{and} \quad \tilde{E}_j = \begin{cases} \{\text{sign}(\tilde{\beta}_j)\} & \text{if } j \in \text{supp}(\tilde{\beta}) \\ [-1, 1] & \text{if } j \notin \text{supp}(\tilde{\beta}). \end{cases}$$

Note that for any two minimizers $\hat{\beta}$ and $\tilde{\beta}$, we have $\hat{\beta}_j \tilde{\beta}_j \geq 0$ for all $j \in [p]$, since otherwise $\check{\beta} = (\hat{\beta} + \tilde{\beta})/2$ satisfies $X\check{\beta} = X\hat{\beta} = X\tilde{\beta}$ as well as $\|\check{\beta}\|_1 < \|\hat{\beta}\|_1 = \|\tilde{\beta}\|_1$, which would lead to a contradiction. We therefore have $\text{supp}(\check{\beta}) = \text{supp}(\hat{\beta}) \cup \text{supp}(\tilde{\beta})$. Note that by a convexity argument, $\check{\beta} \in S_{X, \text{bp}}(y)$ also, so that by (5), there exists $\check{z} \in \mathbb{R}^n$ with $\|X'\check{z}\|_\infty \leq 1$ and $X'_j \check{z} = \text{sign}(\check{\beta}_j)$ for all $j \in \text{supp}(\check{\beta})$. Moreover, $X'\check{z} \in F \cap \tilde{F}$ holds. Now, let F_0 be a face of the face $F \cap \tilde{F}$ of smallest dimension that still intersects $\text{row}(X)$. We write $F_0 = E_{0,1} \times \cdots \times E_{0,p}$ and let $J_0 = \{j \in [p] : |E_{0,j}| = 1\}$. Note that $\text{row}(X)$ must intersect F_0 in its relative interior $\text{relint}(F_0)$ where

$$\text{relint}(F_0) = \text{relint}(E_{0,1}) \times \cdots \times \text{relint}(E_{0,p}) \quad \text{where} \quad \text{relint}(E_{0,j}) = \begin{cases} E_{0,j} & j \in J_0 \\ (-1, 1) & j \notin J_0, \end{cases}$$

since otherwise $\text{row}(X)$ intersects a proper face of F_0 , which contradicts the assumption that F_0 is of minimal dimension. We now need to show that $\text{codim}(F_0) = |J_0| > \text{rk}(X)$. Assume that $|J_0| \leq \text{rk}(X)$. The columns of X_{J_0} are linearly dependent since $X_{J_0} \hat{\beta}_{J_0} = X\hat{\beta} = X\tilde{\beta} = X\check{\beta}$

$X_{J_0}\tilde{\beta}_{J_0}$ with $\hat{\beta}_{J_0} \neq \tilde{\beta}_{J_0}$, since both $\text{supp}(\hat{\beta})$ and $\text{supp}(\tilde{\beta})$ are subsets of $\text{supp}(\check{\beta}) \subseteq J_0$. We therefore have

$$\dim(\text{col}(X_{J_0})) < |J_0| \leq \text{rk}(X) = \dim(\text{col}(X)) \quad \text{and} \quad \text{col}(X)^\perp \subsetneq \text{col}(X_{J_0})^\perp.$$

This implies that we can pick $u \in \text{col}(X_{J_0})^\perp \setminus \text{col}(X)^\perp$ so that $X'_{J_0}u = 0$, but $X'u \neq 0$. Pick $z_0 \in \mathbb{R}^n$ with $X'z_0 \in \text{relint}(F_0)$. The affine line $\{X'(z_0 + tu) : t \in \mathbb{R}\} \subseteq \text{row}(X)$ intersects the relative interior $\text{relint}(F_0)$ and is included in the affine span of F_0 by construction of u . Therefore, by Proposition 14, $\text{row}(X)$ intersects a proper face of F_0 , yielding a contradiction. \blacksquare

B.4.2 CHARACTERIZATION OF PENALIZED MINIMIZERS AND PROOF OF THEOREM 1

In the particular and well-studied case in which the norm of the penalized problem is the ℓ_1 -norm, the solutions to the corresponding optimization problem can be characterized by the Karush-Kuhn-Tucker (KKT) conditions for the LASSO, which can be summarized as follows, see for instance, Bühlmann and Van de Geer (2011).

$$\begin{aligned} \hat{\beta} \in S_{X, \lambda \|\cdot\|_1}(y) &\iff \|X'(y - X\hat{\beta})\|_\infty \leq \lambda \text{ and } X'_j(y - X\hat{\beta}) = \lambda \text{sign}(\hat{\beta}_j) \forall j \in \text{supp}(\hat{\beta}) \quad (6) \\ &\iff \|X'(y - X\hat{\beta})\|_\infty \leq \lambda \text{ and } \hat{\beta}'X'(y - X\hat{\beta}) = \lambda \|\hat{\beta}\|_1 \end{aligned}$$

In the above, the supremum norm is the dual to the ℓ_1 -norm. We can generalize the above characterization for solutions to the penalized problem from (1) in the following proposition. Note that in our notation, the tuning parameter λ is part of the norm $\|\cdot\|$.

Proposition 18 *Let $X \in \mathbb{R}^{n \times p}$, $y \in \mathbb{R}^n$. We have $\hat{\beta} \in S_{X, \|\cdot\|}(y)$ if and only if*

$$\|X'(y - X\hat{\beta})\|^* \leq 1 \text{ and } \hat{\beta}'X'(y - X\hat{\beta}) = \|\hat{\beta}\|.$$

Proof Using subdifferential calculus, the proof is a straightforward consequence of (3) and Proposition 15.

$$\begin{aligned} \hat{\beta} \in S_{X, \|\cdot\|}(y) &\iff 0 \in X'(X\hat{\beta} - y) + \partial_{\|\cdot\|}(\hat{\beta}) \iff X'(y - X\hat{\beta}) \in \partial_{\|\cdot\|}(\hat{\beta}) \\ &\iff \|X'(y - X\hat{\beta})\|^* \leq 1 \text{ and } \hat{\beta}'X'(y - X\hat{\beta}) = \|\hat{\beta}\|. \end{aligned}$$

Before finally showing Theorem 1, the following lemma states that the fitted values are unique over all solutions of the penalized problem for a given y . It is a generalization of Lemma 1 in Tibshirani (2013), who proves this fact for the special case of the LASSO.

Lemma 19 *Let $X \in \mathbb{R}^{n \times p}$, $y \in \mathbb{R}^n$. Then $X\hat{\beta} = X\tilde{\beta}$ for all $\hat{\beta}, \tilde{\beta} \in S_{X, \|\cdot\|}(y)$.*

Proof Assume that $X\hat{\beta} \neq X\tilde{\beta}$ for some $\hat{\beta}, \tilde{\beta} \in S_{X, \|\cdot\|}(y)$ and let $\check{\beta} = (\hat{\beta} + \tilde{\beta})/2$. Because the function $\mu \in \mathbb{R}^n \mapsto \|y - \mu\|_2^2$ is strictly convex, one may deduce that

$$\|y - X\check{\beta}\|_2^2 < \frac{1}{2}\|y - X\hat{\beta}\|_2^2 + \frac{1}{2}\|y - X\tilde{\beta}\|_2^2.$$

Consequently,

$$\frac{1}{2}\|y - X\tilde{\beta}\|_2^2 + \|\tilde{\beta}\| < \frac{1}{2}\left(\frac{1}{2}\|y - X\beta\|_2^2 + \|\beta\| + \frac{1}{2}\|y - X\tilde{\beta}\|_2^2 + \|\tilde{\beta}\|\right),$$

which contradicts both β and $\tilde{\beta}$ being minimizers. \blacksquare

Proof [Proof of Theorem 1]

Throughout the proof, let $B = \text{conv}(V)$ with $V = (V_1 \dots V_k) \in \mathbb{R}^{p \times k}$.

(\Leftarrow) Assume that there exists a face F of B^* that intersects $\text{row}(X)$ (so that F is non-empty) and satisfies $\text{codim}(F) > \text{rk}(X)$ (so that F is proper). This implies that there exists $I \subseteq [k]$ such that

$$F = \{s \in B^* : V_I' s = \mathbf{1}_{|I|}\},$$

where I is the maximal index set satisfying this relationship. Moreover, this implies that $\text{conv}(V_I)$ is a proper, non-empty face of B and that we have $\|s\|^* = 1$ for all $s \in F$ and $\|v\| = 1$ for all $v \in \text{conv}(V_I)$. We show that non-unique solutions exist. Define $\hat{\beta} = \sum_{l \in I} V_l$ and observe that $\|\hat{\beta}\| = |I| \|\sum_{l \in I} V_l / |I|\| = |I|$. Pick $z \in \mathbb{R}^n$ with $X'z \in F$, which exists by assumption, and set $y = X\hat{\beta} + z$. Then $\hat{\beta} \in S_{X, \|\cdot\|}(y)$ by Proposition 18, since

$$\|X'(y - X\hat{\beta})\|^* = \|X'z\|^* = 1 \quad \text{and} \quad \hat{\beta}'(X'(y - X\hat{\beta})) = \hat{\beta}'X'z = \sum_{l \in I} V_l' X'z = |I| = \|\hat{\beta}\|.$$

We now construct $\tilde{\beta} \in S_{X, \|\cdot\|}(y)$ with $\tilde{\beta} \neq \hat{\beta}$. Since $\text{codim}(F_I) = \dim(\text{col}(V_I)) > \text{rk}(X)$, we can pick $h \in \text{col}(V_I) \cap \ker(X)$ with $h \neq 0$. Scale h such that for $h = \sum_{l \in I} c_l V_l$, we have $\max_{l \in I} |c_l| < 1$, and define $\tilde{\beta} = \hat{\beta} + h \neq \hat{\beta}$. Clearly, we have $X\tilde{\beta} = X\hat{\beta}$. Note that $1 + c_l > 0$ and let $\gamma = \sum_{l \in I} (1 + c_l) > 0$. We also have

$$\|\tilde{\beta}\| = \gamma \left\| \sum_{l \in I} \frac{1 + c_l}{\gamma} V_l \right\| = \gamma = \sum_{l \in I} (1 + c_l) = |I| + \sum_{l \in I} c_l (X'z)' V_l = |I| + (X'z)' h = |I| = \|\hat{\beta}\|,$$

proving that $\tilde{\beta} \in S_{X, \|\cdot\|}(y)$ also.

(\Rightarrow) Let us assume that there exists $y \in \mathbb{R}^n$ and $\hat{\beta}, \tilde{\beta} \in S_{X, \|\cdot\|}(y)$ with $\hat{\beta} \neq \tilde{\beta}$. We then have

$$X'(y - X\hat{\beta}) \in \partial_{\|\cdot\|}(\hat{\beta}) \quad \text{and} \quad X'(y - X\tilde{\beta}) \in \partial_{\|\cdot\|}(\tilde{\beta}).$$

Because $X\hat{\beta} = X\tilde{\beta}$ by Lemma 19, one may deduce that $\text{row}(X)$ intersects the face $\partial_{\|\cdot\|}(\hat{\beta}) \cap \partial_{\|\cdot\|}(\tilde{\beta})$. Now, let F^* be a face of $\partial_{\|\cdot\|}(\hat{\beta}) \cap \partial_{\|\cdot\|}(\tilde{\beta})$ of smallest dimension that intersects $\text{row}(X)$ and write

$$F^* = \{s \in B^* : V_I' s = \mathbf{1}_{|I|}\},$$

where I is the largest index set $I \subseteq [k]$ satisfying this relationship. If $\text{codim}(F^*) = \dim(\text{col}(V_I)) \leq \text{rk}(X)$, consider the following. Note that we can pick $u \in \mathbb{R}^n$ for which $X'u \neq 0$ and $X'u \in \text{col}(V_I)^\perp$. For this, let $I_0 \subseteq I$ be such that the columns of V_{I_0} are linearly independent, and $\text{col}(V_{I_0}) = \text{col}(V_I)$. By Lemma 17, we have $\hat{\beta}, \tilde{\beta} \in \text{col}(V_{I_0})$, so that we get

$$XV_{I_0}\gamma = X\hat{\beta} = X\tilde{\beta} = XV_{I_0}\tilde{\gamma}$$

with $\gamma \neq \tilde{\gamma}$, implying that the columns of XV_{I_0} are linearly dependent. But this means that $\text{rk}(XV_I) = \dim(\text{col}(XV_I)) = \dim(\text{col}(XV_{I_0})) < |I_0| = \dim(\text{col}(V_{I_0})) = \dim(\text{col}(V_I)) \leq \text{rk}(X)$.

Therefore, $\text{col}(XV_I) \subsetneq \text{col}(X)$ and, consequently, $\text{col}(X)^\perp \subsetneq \text{col}(XV_I)^\perp$, so that we can pick $u \in \text{col}(XV_I)^\perp \setminus \text{col}(X)^\perp$ for which $X'u \neq 0$ and $X'u \in \text{col}(V_I)^\perp$. Also note that $X'z \in F^*$ for some $z \in \mathbb{R}^n$ and that $X'z$ lies in the relative interior $\text{relint}(F^*)$, as otherwise, $\text{row}(X)$ would intersect a face of $\partial_{\|\cdot\|}(\hat{\beta}) \cap \partial_{\|\cdot\|}(\tilde{\beta})$ of smaller dimension. The affine line $\{X'(z + tu) : t \in \mathbb{R}\} \subseteq \text{row}(X)$ intersects $\text{relint}(F^*)$ and is included in the affine span of F^* by construction. Therefore, by Proposition 14, $\text{row}(X)$ intersects a proper face of F^* , yielding a contradiction. \blacksquare

B.5 Proof of Proposition 3

We turn to proving Proposition 3. Note that a set is negligible with respect to the Lebesgue measure on $\mathbb{R}^{n \times p}$ if and only if it is negligible with respect to the standard Gaussian measure on $\mathbb{R}^{n \times p}$. Therefore, to establish Proposition 3, it suffices to prove the equality

$$\mathbb{P}_Z(\exists y \in \mathbb{R}^n, |S_{Z, \|\cdot\|}(y)| > 1) = 0, \text{ where } Z \in \mathbb{R}^{n \times p} \text{ has iid } \mathcal{N}(0, 1) \text{ entries.} \quad (7)$$

Note that $\text{rk}(Z) = \min\{n, p\}$ almost surely. Therefore, when $n \geq p$, $\ker(Z) = 0$ almost surely and $S_{Z, \|\cdot\|}(y)$ is a singleton almost surely. We use the following lemma to establish (7), where \mathbb{N} stands for the (positive) natural numbers.

Lemma 20 *Let $n \in \mathbb{N}$, $q \geq n + 1$, and $v \in \mathbb{R}^q$ where $v \neq 0$ is a fixed vector. If $Z = (Z_1, \dots, Z_n) \in \mathbb{R}^{q \times n}$ has iid $\mathcal{N}(0, 1)$ entries, then $\mathbb{P}_Z(v \in \text{col}(Z)) = 0$.*

Proof We first prove the result for $q = n + 1$. If $v \in \text{col}(Z)$ then

$$\det(Z_1, \dots, Z_n, v) = 0 \iff \det(Z_1/\|Z_1\|_2, \dots, Z_n/\|Z_n\|_2, v/\|v\|_2) = 0.$$

Now, because the columns $Z_1/\|Z_1\|_2, \dots, Z_n/\|Z_n\|_2$ follow a uniform distribution on the ℓ_2 -unit sphere, we can deduce that the distribution of the random variable $\det(Z_1/\|Z_1\|_2, \dots, Z_n/\|Z_n\|_2, v/\|v\|_2)$ is equal to the distribution of $\det(Z_1/\|Z_1\|_2, \dots, Z_n/\|Z_n\|_2, \zeta/\|\zeta\|_2)$. Here, ζ follows a $\mathbb{N}(0, \mathbb{I}_{n+1})$ distribution, independent from Z_1, \dots, Z_n as conditioning on $\zeta = v$ does not change the distribution. Finally, the random variable

$$\det(Z_1/\|Z_1\|_2, \dots, Z_n/\|Z_n\|_2, \zeta/\|\zeta\|_2) = \frac{1}{\|Z_1\|_2 \times \dots \times \|Z_n\|_2 \times \|\zeta\|_2} \det(Z_1, \dots, Z_n, \zeta)$$

is non-zero almost surely. This implies $\mathbb{P}_Z(v \in \text{col}(Z)) = 0$. When $q > n + 1$, let $I \subseteq [q]$ with $|I| = n + 1$ and $v_I \neq 0$. Consequently, $v_I \in \text{col}(\tilde{Z})$, where $\tilde{Z} \in \mathbb{R}^{(n+1) \times n}$ is obtained by keeping the rows of Z with indices in I . Therefore, $\mathbb{P}_Z(v \in \text{col}(Z)) \leq \mathbb{P}_{\tilde{Z}}(v_I \in \text{col}(\tilde{Z})) = 0$, which concludes the proof. \blacksquare

Proof [Proof of Proposition 3] If $p \leq n$, we are done. If $p > n$, let F_0 be a proper face of B^* such that $\text{codim}(F_0) = q > n$. Note that $0 \notin \text{aff}(F_0)$, the affine space spanned

by F_0 . There exists $A \in \mathbb{R}^{q \times p}$ with orthonormal rows and $v \in \mathbb{R}^q$, $v \neq 0$ such that $\text{aff}(F_0) = \{x \in \mathbb{R}^p : Ax = v\}$. Since $AA' = \mathbb{I}_p$, $AZ' \in \mathbb{R}^{q \times n}$ has iid $\mathcal{N}(0, 1)$ entries. Thus, by Lemma 20, we have

$$\mathbb{P}_Z(\text{row}(Z) \cap F_0 \neq \emptyset) \leq \mathbb{P}_Z(\text{row}(Z) \cap \text{aff}(F_0) \neq \emptyset) = \mathbb{P}_Z(v \in \text{col}(AZ')) = 0. \quad (8)$$

According to Theorem 1 and since $\text{rk}(Z) = n$ almost surely, the following equalities hold.

$$\begin{aligned} \mathbb{P}_Z(\exists y \in \mathbb{R}^n, |S_{Z, \|\cdot\|}(y)| > 1) &= \mathbb{P}_Z\left(\bigcup_{\substack{F \in \mathcal{F}(P) \\ \text{codim}(F) > \text{rk}(Z)}} \{\text{row}(Z) \cap F \neq \emptyset\}\right) \\ &= \mathbb{P}_Z\left(\bigcup_{\substack{F \in \mathcal{F}(P) \\ \text{codim}(F) > n}} \{\text{row}(Z) \cap F \neq \emptyset\}\right) = 0. \end{aligned}$$

The last equality is a consequence of (8). ■

B.6 Proof of Theorem 6

Theorem 6 states that there is a bijection between the SLOPE patterns and the faces of the signed permutahedron. The basis for proving this is the fact that the signed permutahedron is the dual of the sorted- ℓ_1 -norm unit ball, and that any face of it is given by a subdifferential of the sorted- ℓ_1 -norm by Proposition 16.

We start by proving the following proposition which shows that the subdifferential of the sorted- ℓ_1 -norm at zero is, indeed, the signed permutahedron, and also characterizes the subdifferential of the sorted- ℓ_1 -norm for certain values of x .

Proposition 21 *The subdifferential $F_w(x) = \partial_{\|\cdot\|_w}(x)$ of the sorted- ℓ_1 -norm exhibits the following properties.*

- 1) We have $F_w(0) = P_w^\pm$.
- 2) For any $x \in \mathbb{R}^p$ with $x_1 = \dots = x_p > 0$, we have $F_w(x) = P_w$.
- 3) For any $x \in \mathbb{R}^p$ with $x_1 \geq \dots \geq x_k > x_{k+1} \geq \dots \geq x_p \geq 0$, we have

$$F_w(x) = F_{w_{[k]}}(x_{[k]}) \times F_{w_{[k+1:p]}}(x_{[k+1:p]}).$$

- 4) Let $0 < k_1 < \dots < k_l < p$ be an arbitrary subdivision of $[0 : p]$, then for any $x \in \mathbb{R}^p$ with $x_1 = \dots = x_{k_1} > x_{k_1+1} = \dots = x_{k_2} > \dots > x_{k_l+1} = \dots = x_p \geq 0$, we have $\text{codim}(F_w(\text{patt}(x))) = \|\text{patt}(x)\|_\infty$ and

$$F_w(x) = F_w(\text{patt}(x)) = \begin{cases} P_{w_{[k_1]}} \times \dots \times P_{w_{[k_{l-1}+1:k_l]}} \times P_{w_{[k_l+1:p]}} & \text{if } x_p > 0 \\ P_{w_{[k_1]}} \times \dots \times P_{w_{[k_{l-1}+1:k_l]}} \times P_{w_{[k_l+1:p]}}^\pm & \text{if } x_p = 0. \end{cases}$$

Proof 1) By Proposition 15, we may show that $P_w^\pm = B^*$.

(\subseteq) Take any vertex $W = (\sigma_1 w_{\pi(1)}, \dots, \sigma_p w_{\pi(p)})'$ of P_w^\pm and any $x \in \mathbb{R}^p$ with $\|x\|_w \leq 1$. We have

$$W'x = \sum_{j=1}^p \sigma_j w_{\pi(j)} x_j \leq \sum_{j=1}^p |x_j| w_{\pi(j)} \leq \sum_{j=1}^p w_j |x|_{(j)} = \|x\|_w \leq 1$$

and therefore $W \in B^*$. By convexity, $P_w^\pm \subseteq B^*$ follows.

(\supseteq) Let $a'x \leq b_0$ for some $a \in \mathbb{R}^p$ and $b_0 \in \mathbb{R}$ be a valid inequality of P_w^\pm . We show that this is a valid inequality of B^* also: Let W be the vertex of P_w^\pm defined by $W_j = \text{sign}(a_j) w_{\pi^{-1}(j)}$, where the permutation π satisfies $|a_{\pi(1)}| \geq \dots \geq |a_{\pi(p)}|$. For any $s \in B^*$, we have

$$a's \leq \|a\|_w = \sum_{j=1}^p |a_{\pi(j)}| w_j = \sum_{j=1}^p \text{sign}(a_j) a_j w_{\pi^{-1}(j)} = a'W \leq b_0.$$

Since P_w^\pm can be written as the (finite) intersection of half-spaces, $P_w^\pm \supseteq B^*$ follows.

2) According to Proposition 15 and 1), we have

$$F_w(x) = \left\{ s \in P_w^\pm : \sum_{j=1}^p s_j = \sum_{j=1}^p w_j \right\}.$$

A vertex $W = (\sigma_1 w_{\pi(1)}, \dots, \sigma_p w_{\pi(p)})'$ of P_w^\pm with $\sigma \in \{-1, 1\}^p$ and $\pi \in \mathcal{S}_p$ then fulfills $W \in F_w(x)$ if and only if $\sigma_1 = \dots = \sigma_p = 1$. Convexity then yields $F_w(x) = P_w$.

3) (\subseteq) Let $s \in F_w(x)$. We show that $s_{[k]} \in F_{w_{[k]}}(x_{[k]})$ and $s_{[k+1:p]} \in F_{w_{[k+1:p]}}(x_{[k+1:p]})$. Let $e = \frac{x_k - x_{k+1}}{2} > 0$ and $h \in \mathbb{R}^p$ with $\|h\|_\infty < e$. Since the k largest components of $x + h$ are $\{x_j + h_j\}_{j \in [k]}$, we have

$$\|x + h\|_w = \|(x + h)_{[k]}\|_{w_{[k]}} + \|(x + h)_{[k+1:p]}\|_{w_{[k+1:p]}}.$$

Now, take $h \in \mathbb{R}^p$ such that $\|h\|_\infty < e$ and $h_{k+1} = \dots = h_p = 0$. Using the above identity and the definition of $F_w(x)$, one may deduce that

$$\begin{aligned} \|(x + h)_{[k]}\|_{w_{[k]}} &= \|x + h\|_w - \|x_{[k+1:p]}\|_{w_{[k+1:p]}} \\ &\geq \|x\|_w + s'h - \|x_{[k+1:p]}\|_{w_{[k+1:p]}} = \|x_{[k]}\|_{w_{[k]}} + \sum_{j=1}^k s_j h_j. \end{aligned}$$

We therefore obtain that

$$\|x_{[k]} + h\|_{w_{[k]}} \geq \|x_{[k]}\|_{w_{[k]}} + s'_{[k]} h$$

for all $h \in \mathbb{R}^k$ satisfying $\|h\|_\infty < e$. By (4), we conclude $s_{[k]} \in F_{w_{[k]}}(x_{[k]})$. To show that $s_{[k+1:p]} \in F_{w_{[k+1:p]}}(x_{[k+1:p]})$, one can proceed in a similar manner.

(\supseteq) For $s \in F_{w_{[k]}}(x_{[k]}) \times F_{w_{[k+1:p]}}(x_{[k+1:p]})$, we clearly have

$$s'x = \sum_{i=1}^k s_i x_i + \sum_{i=k+1}^p s_i x_i = \|x_{[k]}\|_{w_{[k]}} + \|x_{[k+1:p]}\|_{w_{[k+1:p]}} = \|x\|_w,$$

so that $s \in F_w(x)$ follows.

4) For $x \in \mathbb{R}^p$ with $x_1 = \dots = x_{k_1} > \dots > x_{k_l+1} = \dots = x_p$, $\text{patt}(x)$ is clearly given by

$$\begin{cases} \text{patt}(x)_1 = \dots = \text{patt}(x)_{k_1} = l+1 > \dots > \text{patt}(x)_{k_l+1} = \dots = \text{patt}(x)_p = 1 & \text{if } x_p > 0 \\ \text{patt}(x)_1 = \dots = \text{patt}(x)_{k_1} = l > \dots > \text{patt}(x)_{k_l+1} = \dots = \text{patt}(x)_p = 0 & \text{if } x_p = 0. \end{cases}$$

According to 1), 2) and 3), it is clear that

$$F_w(x) = F_w(\text{patt}(x)) = \begin{cases} P_{w_{[k_1]}} \times \dots \times P_{w_{[k_{l-1}+1:k_l]}} \times P_{w_{[k_l+1:p]}} & \text{if } x_p > 0 \\ P_{w_{[k_1]}} \times \dots \times P_{w_{[k_{l-1}+1:k_l]}} \times P_{w_{[k_l+1:p]}^\pm} & \text{if } x_p = 0. \end{cases}$$

Since the codimension of a permutahedron is equal to 1 (see Maes and Kappen, 1992; Simion, 1997), the one of signed permutahedron is equal to 0, and since the (co-)dimensions of the individual (sign) permutahedra can simply be added up, we have $\text{codim}(F_w(x)) = \|\text{patt}(x)\|_\infty$. \blacksquare

Proposition 21 lays the groundwork by essentially proving Theorem 6 for all SLOPE patterns with non-negative and non-decreasing components. We denote this set of patterns by $\mathcal{P}_p^{\geq,+}$, given by

$$\mathcal{P}_p^{\geq,+} = \{m \in \mathcal{P}_p : m_1 \geq \dots \geq m_p \geq 0\}.$$

In order to extend this proposition to all SLOPE patterns in \mathcal{P}_p , we introduce the following group of linear transformations.

Definition 22 Let $\sigma \in \{-1, 1\}^p$, let $\pi \in \mathcal{S}_p$. We define the map

$$\phi_{\sigma,\pi} : x \in \mathbb{R}^p \mapsto (\sigma_1 x_{\pi(1)}, \dots, \sigma_p x_{\pi(p)})'$$

and denote by $\mathcal{G} = \{\phi_{\sigma,\pi} : \sigma \in \{-1, 1\}^p, \pi \in \mathcal{S}_p\}$.

The set \mathcal{G} is a finite sub-group of the group of orthogonal transformations on \mathbb{R}^p . We list a number of straight-forward properties of \mathcal{G} in the following lemma.

Lemma 23 Let $x, v \in \mathbb{R}^p$, $\phi \in \mathcal{G}$, and let $\sigma \in \{-1, 1\}^p$ and $\pi \in \mathcal{S}_p$. Then the following holds.

- 1) $x'v = \phi(x)'\phi(v)$
- 2) $\|x\|_w = \|\phi(x)\|_w$
- 3) $\|x\|_\infty = \|\phi(x)\|_\infty$
- 4) $\phi(\mathcal{P}_p) = \mathcal{P}_p$ and $\phi(P_w^\pm) = P_w^\pm$
- 5) $\text{patt}(\phi(x)) = \phi(\text{patt}(x))$
- 6) $\phi_{\sigma,\pi}^{-1} = \phi_{\sigma,\pi^{-1}} \in \mathcal{G}$

7) If, for $m \in \mathcal{P}_p$, $|m_{\pi(1)}| \geq \dots \geq |m_{\pi(p)}|$ and $\sigma_j m_{\pi(j)} = |m_{\pi(j)}|$ for all $j \in [p]$, then $\phi_{\sigma, \pi}(m) \in \mathcal{P}_p^{\geq, +}$.

Lemma 24 Let $\phi \in \mathcal{G}$ and $x \in \mathbb{R}^p$. We then have

$$\phi^{-1}(F_w(\phi(x))) = F_w(x) \quad \text{and} \quad F_w(\phi(x)) = \phi(F_w(x)).$$

Proof The two statements are equivalent, we show the second one. Let $s \in P_w^\pm$. Then

$$\begin{aligned} s \in F_w(\phi(x)) &\iff s' \phi(x) = \|\phi(x)\|_w \iff \phi^{-1}(s)' x = \|x\|_w \\ &\iff \phi^{-1}(s) \in F_w(x) \iff s \in \phi(F_w(x)) \end{aligned}$$

by Proposition 15 and Lemma 23. ■

We are now equipped to prove Theorem 6.

Proof [Proof of Theorem 6]

We start by proving 1) and 2) before showing that the map is a bijection.

1) Let $m \in \mathcal{P}_p$ and let $\phi \in \mathcal{G}$ such that $\phi(m) \in \mathcal{P}_p^{\geq, +}$. According to Lemma 24, and because ϕ is an isomorphism on \mathbb{R}^p , we have

$$\text{codim}(F_w(m)) = \text{codim}(\phi^{-1}(F_w(\phi(m)))) = \text{codim}(F_w(\phi(m))) = \|\phi(m)\|_\infty = \|m\|_\infty.$$

2) Let $x \in \mathbb{R}^p$ and let $\phi \in \mathcal{G}$ such that $\phi(x)_1 \geq \dots \geq \phi(x)_p \geq 0$. According to Lemma 24 and Proposition 21, the following equalities hold

$$F_w(x) = \phi^{-1}(F_w(\phi(x))) = \phi^{-1}(F_w(\text{patt}(\phi(x)))) = \phi^{-1}(F_w(\phi(\text{patt}(x)))) = F_w(\text{patt}(x)).$$

We now show that the mapping under consideration is indeed a bijection between \mathcal{P}_p and \mathcal{F}_0 .

(surjection) According to Proposition 16, a non-empty face of P_w^\pm can be expressed as $F_w(x)$ for some $x \in \mathbb{R}^p$. According to 2) above, we have $F_w(x) = F_w(\text{patt}(x))$ for $\text{patt}(x) \in \mathcal{P}_p$.

(injection) Note that Proposition 21 shows that the mapping is injective on $\mathcal{P}_p^{\geq, +}$. To prove that it remains injective on all of \mathcal{P}_p , we show that $|\mathcal{P}_p| \leq |\mathcal{F}_0|$. For this, we need several definitions. For $m \in \mathcal{P}_p$, let $\text{stab}_{\mathcal{G}}(m) = \{\phi \in \mathcal{G} : \phi(m) = m\}$ and $\text{orb}_{\mathcal{G}}(m) = \{\phi(m) : \phi \in \mathcal{G}\}$, the stabilizer and orbit of m , respectively, with respect to \mathcal{G} . For $m \in \mathcal{P}_p$, there exists $\phi \in \mathcal{G}$ such that $\phi(m) \in \mathcal{P}_p^{\geq, +}$. Therefore, the orbit-stabilizer formula (Artin, 2011)[Proposition 6.8.4] gives

$$\mathcal{P}_p = \bigcup_{m \in \mathcal{P}_p^{\geq, +}} \text{orb}_{\mathcal{G}}(m) \implies |\mathcal{P}_p| \leq \sum_{m \in \mathcal{P}_p^{\geq, +}} |\text{orb}_{\mathcal{G}}(m)| = \sum_{m \in \mathcal{P}_p^{\geq, +}} \frac{|\mathcal{G}|}{|\text{stab}_{\mathcal{G}}(m)|}.$$

We also look at stabilizer and orbit when \mathcal{G} operates on \mathcal{F}_0 . For a face $F \in \mathcal{F}_0$, let $\text{stab}_{\mathcal{G}}(F) = \{\phi \in \mathcal{G} : \phi(F) = F\}$ and $\text{orb}_{\mathcal{G}}(F) = \{\phi(F) : \phi \in \mathcal{G}\}$. We first show that if $\text{orb}_{\mathcal{G}}(F_w(m)) \cap \text{orb}_{\mathcal{G}}(F_w(\tilde{m})) \neq \emptyset$ for some $m, \tilde{m} \in \mathcal{P}_p^{\geq, +}$, $m = \tilde{m}$ follows. Let us assume

that $F_w(\tilde{m}) = \phi(F_w(m))$ for some $\phi \in \mathcal{G}$. Note that $\phi(F_w(m)) = F_w(\phi(m))$ by Lemma 24. Since $w \in F_w(m)$ and $w \in F_w(\tilde{m}) = F_w(\phi(m))$, we have

$$w'm = \|m\|_w = \|\phi(m)\|_w = w'\phi(m),$$

where the first equality holds since $m \in \mathcal{P}_p^{\geq,+}$, the second equality holds by Lemma 23 and the last equality holds since $m \in F_w(\phi(m))$. Now, if $\phi(m) \neq m$, $w'\phi(m) < \|m\|_w$ follows since the components of w are positive and strictly decreasing. But that would contradict the above, so $\phi(m) = m$ must hold. Consequently, $F_w(\tilde{m}) = F_w(m)$, which in turn implies $\tilde{m} = m$ by Proposition 21.

Now, let $m \in \mathcal{P}_p^{\geq,+}$ and let us show that $\text{stab}_{\mathcal{G}}(m) = \text{stab}_{\mathcal{G}}(F_w(m))$. The inclusion $\text{stab}_{\mathcal{G}}(m) \subseteq \text{stab}_{\mathcal{G}}(F_w(m))$ immediately follows from

$$\begin{aligned} \phi \in \text{stab}_{\mathcal{G}}(m) &\implies F_w(m) = \phi^{-1}(F_w(\phi(m))) = \phi^{-1}(F_w(m)) \implies \phi(F_w(m)) = F_w(m) \\ &\implies \phi \in \text{stab}_{\mathcal{G}}(F_w(m)). \end{aligned}$$

To show $\text{stab}_{\mathcal{G}}(F_w(m)) \subseteq \text{stab}_{\mathcal{G}}(m)$, let $\phi \in \text{stab}_{\mathcal{G}}(F_w(m))$ and note that $F_w(m) = \phi(F_w(m)) = F_w(\phi(m))$. Since $m \in \mathcal{P}_p^{\geq,+}$, this implies that $w \in F_w(m) = F_w(\phi(m))$, so that the same reasoning as above yields $m = \phi(m)$ and $\phi \in \text{stab}_{\mathcal{G}}(m)$.

To conclude, note that since the orbits $\text{orb}_{\mathcal{G}}(F_w(m))$ with $m \in \mathcal{P}_p^{\geq,+}$ are disjoint, and since $\text{stab}_{\mathcal{G}}(m) = \text{stab}_{\mathcal{G}}(F_w(m))$, we may deduce that

$$|\mathcal{P}_p| \leq \sum_{m \in \mathcal{P}_p^{\geq,+}} \frac{|\mathcal{G}|}{|\text{stab}_{\mathcal{G}}(F_w(m))|} = \sum_{m \in \mathcal{P}_p^{\geq,+}} |\text{orb}_{\mathcal{G}}(F_w(m))| = \left| \bigcup_{m \in \mathcal{P}_p^{\geq,+}} \text{orb}_{\mathcal{G}}(F_w(m)) \right| \leq |\mathcal{F}_0|. \quad \blacksquare$$

B.7 Proof of Theorem 8

The following lemma generalizes Proposition 4.1 from Gilbert (2017) that is stated for the ℓ_1 -norm to an arbitrary norm. This lemma is used in the proof of both Theorem 8 and Theorem 13.

Lemma 25 *Let $s \in \mathbb{R}^p$ and $\|\cdot\|$ be a norm on \mathbb{R}^p . The vector space $\text{row}(X)$ intersects $\partial_{\|\cdot\|}(s)$ if and only if the following holds.*

$$Xb = Xs \implies \|b\| \geq \|s\| \tag{9}$$

Proof Consider the function $f_s : \mathbb{R}^p \rightarrow \{0, \infty\}$ given by

$$f_s(b) = \begin{cases} 0 & Xb = Xs \\ \infty & \text{else.} \end{cases}$$

Then (9) holds for b if and only if s is a minimizer of the function $b \mapsto \|b\| + f_s(b)$. Since we have $\partial_{f_s}(b) = \text{row}(X)$ whenever $Xb = Xs$, we can deduce that the implication (9) occurs if and only if

$$0 \in \text{row}(X) + \partial_{\|\cdot\|}(s) \iff \text{row}(X) \cap \partial_{\|\cdot\|}(s) \neq \emptyset.$$

■

Proof [Proof of Theorem 8] (\implies) If m is an accessible SLOPE pattern, then

$$\exists y \in \mathbb{R}^n, \exists \hat{\beta} \in S_{X, \|\cdot\|_w}(y) \text{ such that } \text{patt}(\hat{\beta}) = m.$$

By Theorem 6, we may deduce that $\partial_{\|\cdot\|_w}(\hat{\beta}) = F_w(\hat{\beta}) = F_w(m)$. Consequently,

$$0 \in X'(X\hat{\beta} - y) + \partial_{\|\cdot\|_w}(\hat{\beta}) \implies X'(y - X\hat{\beta}) \in F_w(m).$$

Therefore, $\text{row}(X)$ intersects $F_w(m)$ (geometric characterization), or, equivalently, by Lemma 25, whenever $Xb = Xm$ we have $\|b\|_w \geq \|m\|_w$ (analytic characterization).

(\impliedby) If $\text{row}(X)$ intersects the face $F_w(m)$ (geometric characterization), or, equivalently, whenever $Xb = Xm$ we have $\|b\|_w \geq \|m\|_w$ (analytic characterization), there exists $z \in \mathbb{R}^n$ such that $X'z = f \in F_w(m)$. We set $y = z + Xm$ and show that $m \in S_{X, \|\cdot\|_w}(y)$. We have

$$\|X'(y - Xm)\|_w^* = \|f\|_w^* \leq 1 \text{ and } m'X'(y - Xm) = m'f = \|m\|_w,$$

which, by Proposition 18, yields $m \in S_{X, \|\cdot\|_w}(y)$. ■

B.8 Proof of Proposition 10

Proof By Theorem 8, we know that

$$m \in \mathcal{P}_p \text{ is accessible} \iff \text{row}(X) \cap F_w(m) \neq \emptyset \iff \exists f \in \mathbb{R}^n : X'f \in F_w(m) \iff f \in N_w(m),$$

which proves the first statement. Now, let $y = f + Xb$, where $f \in N_w(m)$ and $b \in \mathbb{R}^p$ such that $\text{patt}(b) = m$. Note that

$$\|X'(y - Xb)\|_w^* = \|X'f\|_w^* \leq 1 \text{ and } b'X'(y - Xb) = b'X'f = \|b\|_w^*,$$

where the first inequality holds since $X'f \in F_w(m)$, a face of P_w^\pm , and the latter one by applying Proposition 16 after noticing that $X'f \in F_w(m) = F_w(b) = \partial_{\|\cdot\|_w}(b)$ by Theorem 6. Proposition 18 then yields $b \in S_{X, \|\cdot\|_w}(y)$, so that $y \in A_w(m)$.

Conversely, let $y \in A_w(m)$ and let $\hat{\beta} \in S_{X, \|\cdot\|_w}(y)$ so that $\text{patt}(\hat{\beta}) = m$. Then $y - X\hat{\beta} \in N_w(m)$ since by Proposition 18, we have

$$X'(y - X\hat{\beta}) \in \partial_{\|\cdot\|_w}(\hat{\beta}) = F_w(m),$$

where the last equality holds by Theorem 6. ■

B.9 Proof of Proposition 11

Proof Note that by Proposition 18 we have that $\hat{\beta} \in S_{X, \|\cdot\|}(y)$ if and only if we have

$$\|X'(y - X\hat{\beta})\|^* \leq 1 \text{ and } \hat{\beta}'(y - X\hat{\beta}) = \|\hat{\beta}\|.$$

Consequently, when $\|X'u\|^* \leq 1$ it is clear that $0 \in S_{X, \|\cdot\|}(u)$ implying that $S_{X, \|\cdot\|}(u) = \{0\}$ as all elements of $S_{X, \|\cdot\|}(u)$ must have the same norm. Now, let $u \in A_\emptyset$ and remember that $\hat{u} = y - X\hat{\beta}$. The following inequality

$$(y - \hat{u})'(u - \hat{u}) = \underbrace{\hat{\beta}'X'u}_{\leq \|\hat{\beta}\|} - \underbrace{\hat{\beta}'X'(y - X\hat{\beta})}_{=\|\hat{\beta}\|} \leq 0$$

shows that, indeed, \hat{u} is the projection of y onto the convex null set A_\emptyset . ■

B.10 Proof of Theorem 13

Proof (\implies) Let σ be an accessible sign vector for LASSO. Then there exists $y \in \mathbb{R}^n$ and $\hat{\beta} \in S_{X, \lambda \|\cdot\|_1}(y)$ such that $\text{sign}(\hat{\beta}) = \sigma$. According to the characterization of LASSO minimizers in (6), by setting $z = (y - X\hat{\beta})/\lambda$, one may deduce that $X'z \in F_1(\sigma)$. If σ is an accessible sign vector for BP, there exists $y \in \text{col}(X)$ and $\hat{\beta} \in S_{X, \text{bp}}(y)$ with $\text{sign}(\hat{\beta}) = \sigma$. According to the characterization of BP minimizers in (5), there exists $z \in \mathbb{R}^n$ such that $X'z \in F_1(\sigma)$. Therefore, $\text{row}(X)$ intersects $F_1(\sigma) = \partial_{\|\cdot\|_1}(\sigma)$ (geometric characterization), or, equivalently, by Lemma 25, whenever $Xb = X\sigma$, we have $\|b\|_1 \geq \|\sigma\|_1$ (analytic characterization).

(\impliedby) If $\text{row}(X)$ intersects the face $F_1(\sigma)$ (geometric characterization) or, equivalently, if $Xb = X\sigma$ implies $\|b\|_1 \geq \|\sigma\|_1$ (analytic characterization), then there exists $f \in F_1(\sigma)$ and $z \in \mathbb{R}^n$ such that $X'z = f$. Note that $j \in \text{supp}(\sigma)$ implies that $f_j = \sigma_j = \text{sign}(\sigma_j)$. Set $y = \lambda z + X\sigma$. We show that $\sigma \in S_{X, \lambda \|\cdot\|_1}(y)$. We have

$$\begin{cases} \|X'(y - X\sigma)\|_\infty = \lambda \|X'z\|_\infty \leq \lambda, \\ X'_j(y - X\sigma) = \lambda X'_j z = \lambda f_j = \lambda \sigma_j = \lambda \text{sign}(\sigma_j) \quad \forall j \in \text{supp}(\sigma), \end{cases}$$

so that according to the characterization of LASSO minimizers in (6), we have $\sigma \in S_{X, \lambda \|\cdot\|_1}(y)$, implying that σ is accessible for LASSO. For BP, set $y = X\sigma$ and note that, according to the characterization of BP minimizers in (5), $\sigma \in S_{X, \text{bp}}(y)$, implying that σ is also accessible for BP. ■

Corollary 26 *Let $X \in \mathbb{R}^{n \times p}$, $\sigma \in \{-1, 0, 1\}^p$ and assume that $\hat{\beta}$ is the unique solution to the BP problem $S_{X, \text{bp}}(y)$ with $y = X\sigma$. Let $\tilde{\beta} \in \mathbb{R}^p$ satisfy $\|\tilde{\beta} - \hat{\beta}\|_\infty < 1/2$. We then have that*

$$\sigma \text{ is accessible} \iff \text{sign}(\text{round}(\tilde{\beta})) = \sigma,$$

where $\text{round}(\cdot)$ rounds componentwise to the nearest integer.

Proof (\implies) If σ is accessible, by the analytic characterization in Theorem 13, $\hat{\beta} = \sigma$. Since $\|\tilde{\beta} - \sigma\|_\infty < 1/2$, we get $\text{sign}(\text{round}(\tilde{\beta})) = \text{round}(\tilde{\beta}) = \sigma$.

(\impliedby) If σ is not accessible, we have $\text{sign}(\hat{\beta}) \neq \sigma$. Using $\|\tilde{\beta} - \hat{\beta}\|_\infty < 1/2$, we can show that

$$F_1(\text{sign}(\hat{\beta})) = \partial_{\|\cdot\|_1}(\text{sign}(\hat{\beta})) \subseteq \partial_{\|\cdot\|_1}(\text{sign}(\text{round}(\tilde{\beta}))) = F_1(\text{sign}(\text{round}(\tilde{\beta}))).$$

Since $\text{row}(X)$ intersects $F_1(\text{sign}(\hat{\beta}))$ by the geometric characterization in Theorem 13, $\text{sign}(\text{round}(\tilde{\beta}))$ is accessible. But then $\text{sign}(\text{round}(\tilde{\beta})) \neq \sigma$ must hold. \blacksquare

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