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► **To cite this version:**

Patrick J C Tardivel, Rémi Servien, Didier Concordet. Simple expressions of the LASSO and SLOPE estimators in low-dimension. *Statistics*, 2020, 10.1080/02331888.2020.1720019 . hal-01755076v3

HAL Id: hal-01755076

<https://hal.science/hal-01755076v3>

Submitted on 19 Dec 2019

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Simple expressions of the LASSO and SLOPE estimators in low-dimension

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ARTICLE HISTORY

Compiled December 19, 2019

The final version of this article will be published in Statistics.

ABSTRACT

We study the LASSO and SLOPE estimators when the design X satisfies $\ker(X) = \mathbf{0}$. Similarly to the LASSO, the SLOPE estimator has an explicit expression when the design matrix X is orthogonal which is reported in the main theorem of this article. We state that, even if the design is not orthogonal, even if residuals are correlated, up to a transformation, the LASSO and SLOPE estimators have a simple expression based on the Best Linear Unbiased Estimator (BLUE). Comparisons with the LASSO estimator show the benefits of the soft-thresholded BLUE.

KEYWORDS

Best linear unbiased estimator; LASSO; SLOPE

1. Introduction

Let us consider the following low-dimensional linear model

$$Y = X\beta^* + \varepsilon, \tag{1}$$

where X is a $n \times p$ fixed design matrix with $\ker(X) = \mathbf{0}$ (*i.e.* $n \geq p$), $\beta^* \in \mathbb{R}^p$ is an unknown parameter and ε is a centered random vector with an invertible and known covariance matrix Γ .

The Least Absolute Shrinkage and Selection Operator (LASSO) estimator and the Sorted L-One Penalized Estimation (SLOPE) estimator respectively introduced by Tibshirani [1] and Bogdan et al. [2] are defined by

$$\hat{\beta}^{\text{lasso}} := \operatorname{argmin}_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{2} \|Y - X\beta\|^2 + \lambda \|\beta\|_1 \right\} \text{ and,} \tag{2}$$

$$\hat{\beta}^{\text{slope}} := \operatorname{argmin}_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{2} \|Y - X\beta\|^2 + \lambda_1 |\beta_{[1]}| + \cdots + \lambda_p |\beta_{[p]}| \right\}. \tag{3}$$

In the second expression, the tuning parameters $(\lambda_i)_{1 \leq i \leq p}$ satisfy $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$. The brackets $[\cdot]$ denote a permutation of $\{1, \dots, p\}$ such that $|\beta_{[1]}| \geq \dots \geq |\beta_{[p]}|$.

It is well known that when the design X is orthogonal (*i.e.* $X'X = Id_p$), the LASSO estimator leads to the following soft-thresholded Ordinary Least Squares (OLS) estimator [1]

$$\hat{\beta}^{\text{lasso}} = \left(\text{sign}(\hat{\beta}_1^{\text{ols}})(|\hat{\beta}_1^{\text{ols}}| - \lambda)_+, \dots, \text{sign}(\hat{\beta}_p^{\text{ols}})(|\hat{\beta}_p^{\text{ols}}| - \lambda)_+ \right). \quad (4)$$

Popularized by the pioneer work of Tibshirani, the orthogonal design became a case study [3–8]. Furthermore some properties such as the irrepresentable condition [9–12] hold when X is orthogonal. The orthogonal design is also a case study for the SLOPE estimator [2,13,14].

Whatever the considered estimator, the orthogonal design setting appears to be an ideal case. When we tried to generalize its properties to the non-orthogonal setting, we discovered a relevant orthogonalizing transformation $U_s := D(X'\Gamma^{-1}X)^{-1}X'\Gamma^{-1}$, where $s := (s_1, \dots, s_p)$, $s_1 > 0, \dots, s_p > 0$ and $D := \text{diag}(1/\sqrt{s_1}, \dots, 1/\sqrt{s_p})$. Actually, if we consider the new model $\tilde{Y} = \tilde{X}\beta^* + \tilde{\varepsilon}$, where $\tilde{Y} = U_s Y$, $\tilde{X} = U_s X$ and $\tilde{\varepsilon} = U_s \varepsilon$, the LASSO estimator $\tilde{\beta}^s$ after applying the transformation U_s can simply be written as a function of the Best Linear Unbiased Estimator (BLUE) in the following way:

$$\tilde{\beta}^s := \underset{\beta \in \mathbb{R}^p}{\text{argmin}} \left\{ \frac{1}{2} \left\| \tilde{Y} - \tilde{X}\beta \right\|^2 + \lambda \|\beta\|_1 \right\} \Leftrightarrow \tilde{\beta}^s = \left(\text{sign}(\hat{\beta}_i^{\text{blue}})(|\hat{\beta}_i^{\text{blue}}| - \lambda s_i)_+ \right)_{1 \leq i \leq p}. \quad (5)$$

Similarly to the LASSO estimator, we also obtained a simple expression for the SLOPE estimator based on the BLUE. We can notice that, in low-dimension, the U_s transformation giving (5) does not require X to be orthogonal or the components of ε to be independent; but $\ker(X) = \mathbf{0}$ is necessary.

1.1. Notations

In this article, we denote J the SLOPE norm $J : \beta \in \mathbb{R}^p \mapsto \lambda_1 |\beta_{[1]}| + \dots + \lambda_p |\beta_{[p]}|$ where $|\beta_{[1]}| \geq \dots \geq |\beta_{[p]}|$ and $\lambda_1 \geq \dots \geq \lambda_p$ (see for example [2] for the proof that J is a norm). The OLS and BLUE estimators of the model (1), denoted $\hat{\beta}^{\text{ols}}$ and $\hat{\beta}^{\text{blue}}$, are respectively equal to

$$\hat{\beta}^{\text{ols}} := (X'X)^{-1}X'Y \quad \text{and} \quad \hat{\beta}^{\text{blue}} := (X'\Gamma^{-1}X)^{-1}X'\Gamma^{-1}Y. \quad (6)$$

Whatever $t \in \mathbb{R}$, we set $(t)_+ = \max\{t, 0\}$ and $\text{sign}(t) = \mathbf{1}_{t>0} - \mathbf{1}_{t<0}$. Given a subset $A \subset \mathbb{R}^p$, $\text{conv}(A)$ is the smallest convex set containing A . Finally, the notation Id_p represents the $p \times p$ identity matrix.

2. Orthogonalization of the design: simple form of the LASSO and SLOPE

When the design is orthogonal, some algorithms provide the SLOPE estimation [2] but the estimator writing is not explicit. To our knowledge, there does not exist currently

any explicit formula for the SLOPE. In the following theorem, we provide the explicit expression of the SLOPE when X is orthogonal.

Theorem 2.1. *Let τ be a permutation of $\{1, \dots, p\}$ ordering the components of the OLS estimator (6) namely $|\hat{\beta}_{\tau(1)}^{\text{ols}}| \geq \dots \geq |\hat{\beta}_{\tau(p)}^{\text{ols}}|$. Let $(\hat{S}_k)_{1 \leq k \leq p}$ be a sequence defined by $\forall k \in \{1, \dots, p\}, \hat{S}_k := \sum_{i=1}^k (|\hat{\beta}_{\tau(i)}^{\text{ols}}| - \lambda_i)$ and let $1 \leq k_1 \leq \dots \leq k_s = p$ be a partition of $\{1, \dots, p\}$ such that*

$$k_1 = \max \left\{ \operatorname{argmax}_{k \in \{1, \dots, p\}} \left\{ \frac{\hat{S}_k}{k} \right\} \right\} \text{ and } \forall i \in \{2, \dots, s\}, k_i = \max \left\{ \operatorname{argmax}_{k > \hat{k}_{i-1}} \left\{ \frac{\hat{S}_k - \hat{S}_{k_{i-1}}}{k - \hat{k}_{i-1}} \right\} \right\}.$$

When the design matrix X is orthogonal, whatever $i \in \{1, \dots, p\}$, the components of $\hat{\beta}^{\text{slope}}$ (2) satisfy the inequality $\hat{\beta}_i^{\text{ols}} \hat{\beta}_i^{\text{slope}} \geq 0$ and $(|\hat{\beta}_{\tau(1)}^{\text{slope}}|, \dots, |\hat{\beta}_{\tau(p)}^{\text{slope}}|)$ is given by

$$\underbrace{\left(\left(\frac{\hat{S}_{k_1}}{k_1} \right)_+ , \dots , \left(\frac{\hat{S}_{k_1}}{k_1} \right)_+ \right)}_{k_1 \text{ components}} , \dots , \underbrace{\left(\frac{\hat{S}_{k_s} - \hat{S}_{k_{s-1}}}{k_s - k_{s-1}} \right)_+ , \dots , \left(\frac{\hat{S}_{k_s} - \hat{S}_{k_{s-1}}}{k_s - k_{s-1}} \right)_+ \right)}_{k_s - k_{s-1} \text{ components}}.$$

Let us notice that when $\hat{\beta}^{\text{ols}}$ has a continuous distribution over \mathbb{R}^p , the Cesàro sequence (\hat{S}_k/k) almost surely reaches its maximum at a unique point. In other terms, $k_1 := \operatorname{argmax} \{\hat{S}_k/k\}$ is unique and the same argument applies for k_2, \dots, k_s . When $\lambda_1 = \dots = \lambda_p = \lambda$, the Cesàro sequence is non-increasing and consequently the following equality holds

$$\forall i \in \{1, \dots, p\}, \hat{\beta}_i^{\text{slope}} = \operatorname{sign}(\hat{\beta}_i^{\text{ols}}) (|\hat{\beta}_i^{\text{ols}}| - \lambda)_+ = \hat{\beta}_i^{\text{lasso}}.$$

As a consequence, when $\lambda_1 = \dots = \lambda_p = \lambda$ in the orthogonal setting, the formula of the SLOPE given in the theorem 2.1 coincides with the one of the LASSO given in (4).

Remark: When X is orthogonal, $\varepsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2 Id_n)$ and $\lambda_i = \sigma z(1 - iq/(2p)), i \in \{1, \dots, p\}$ (where $q \in (0, 1)$ and $z(\eta)$ is the η -quantile of the $\mathcal{N}(0, 1)$ distribution), the procedure rejecting the null hypothesis $\beta_i^* = 0$ when $\hat{\beta}_i^{\text{slope}} \neq 0$ controls the FDR at level q [2]. The explicit expression of the SLOPE shows that this procedure is close to the original Benjamini-Hochberg procedure [15] (actually, these procedures are equal when the sequence (\hat{S}_k/k) is decreasing) and this provides an intuitive explanation for the FDR control.

An illustration of the relationship between the OLS estimator and the SLOPE estimator when X is orthogonal is given by the figure 1 in the special case where $p = 2$, $\lambda_1 = 2$ and $\lambda_2 = 1$.

This figure also illustrates the properties of the SLOPE: this estimator is sparse (*i.e.* some components are exactly equal to 0), and some components are equal in absolute value.

Remarks: Let us point out some relevant transformations allowing us to obtain simple expressions for the LASSO estimator and the SLOPE:

- **Transformation which brings back to the orthogonal setting:** When

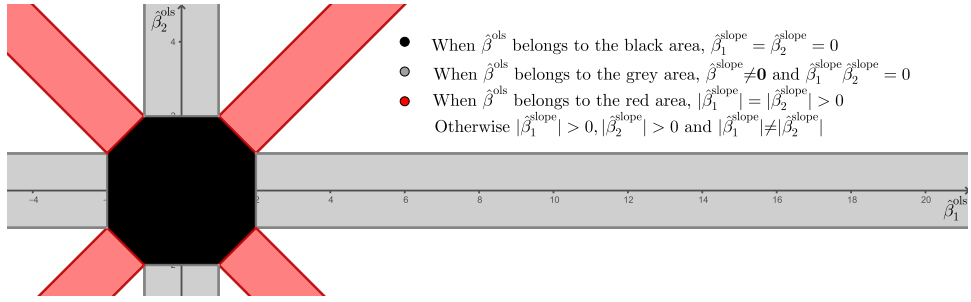


Figure 1. This figure illustrates the relationship between the OLS estimator and the SLOPE, the x-axis and y-axis represent respectively the first and second component of the OLS estimator. Let \hat{S}_1, \hat{S}_2 be defined as in the theorem 2.1. When $\hat{S}_1 \leq 0$ and $\hat{S}_2 \leq 0$ then $\hat{\beta}^{\text{ols}}$ is on the black area and $\hat{\beta}^{\text{slope}} = \mathbf{0}$. When $\hat{S}_1 \leq \hat{S}_2/2$ and $\hat{S}_2/2 > 0$ then $\hat{\beta}^{\text{ols}}$ is on the red area and $|\hat{\beta}_1^{\text{slope}}| = |\hat{\beta}_2^{\text{slope}}| > 0$. When $\hat{S}_1 > \hat{S}_2/2$ with $\hat{S}_1 > 0$ and $\hat{S}_2 - \hat{S}_1 < 0$ then $\hat{\beta}^{\text{ols}}$ is on the grey area, $\hat{\beta}^{\text{slope}} \neq \mathbf{0}$ and $|\hat{\beta}_1^{\text{slope}}| |\hat{\beta}_2^{\text{slope}}| = 0$. Otherwise $\hat{\beta}^{\text{ols}}$ is on the white area then $|\hat{\beta}_1^{\text{slope}}| > 0, |\hat{\beta}_2^{\text{slope}}| > 0$ and $|\hat{\beta}_1^{\text{slope}}| \neq |\hat{\beta}_2^{\text{slope}}|$.

X is not orthogonal, applying the transformation $U_1 := (X'\Gamma^{-1}X)^{-1}X'\Gamma^{-1}$ on each side of the model (1) brings back the orthogonal setting in which $\tilde{Y} := \beta^* + \tilde{\varepsilon}$, where $\tilde{Y} = U_1Y$ and $\tilde{\varepsilon} = U_1\varepsilon$. In this new model, the LASSO estimator has the expression described in (5) with $s_1 = \dots = s_p = 1$ and the SLOPE has the expression described in the theorem 2.1 except that the OLS estimator is substituted by the more accurate BLUE estimator.

- **Transformation which brings back the orthogonal columns setting:** When columns of X are not orthogonal (*i.e.* when $X'X$ is not diagonal), applying the transformation $U_s := D(X'\Gamma^{-1}X)^{-1}X'\Gamma^{-1}$, where $s := (s_1, \dots, s_p)$, $s_1 > 0, \dots, s_p > 0$ and $D := \text{diag}(1/\sqrt{s_1}, \dots, 1/\sqrt{s_p})$, on each side of the model (1) returns the orthogonal columns' setting. After applying this transformation, LASSO's expression is still explicit and its expression is described by formula (5).

To avoid confusion, we call soft-thresholded BLUE the LASSO-type estimator whose formula is given in (5) and LASSO the estimator solution of (2). The soft-thresholded BLUE is easier to compute than the LASSO estimator (because the LASSO estimator computation needs to solve numerically the optimization problem described in (2)) and the soft-thresholded BLUE estimator is also easier to interpret than the LASSO estimator (contrarily to the LASSO estimator, the relationship between BLUE and the soft-thresholded BLUE is explicit). Thus it is recommended that in low-dimension the soft-thresholded BLUE should be used instead of the LASSO estimator, except if there are particular reasons for using the latter. Finally, from procedures based on the LASSO estimator defined in (2) one can derive new procedures based on the soft-thresholded BLUE given in (5) as illustrated in the following remark.

Remark: Janson and Su [16] have developed a multiple testing procedure based on the knockoff-LASSO estimator defined as follows

$$\hat{\beta}^{\text{kn-lasso}} := \underset{\beta \in \mathbb{R}^p}{\text{argmin}} \frac{1}{2} \|Y - X_{\text{ko}}\beta\|^2 + \lambda \|\beta\|_1.$$

Since the matrix X_{ko} (defined in Barber and Candès [17]) satisfies $\ker(X_{\text{ko}}) = \mathbf{0}$, up

to a transformation, the knockoff-LASSO is just a soft-thresholded BLUE (where the BLUE is $(X'_{\text{ko}}\Gamma^{-1}X_{\text{ko}})^{-1}X_{\text{ko}}\Gamma^{-1}Y$, with $\Gamma = \text{var}(Y)$). Therefore, from the procedure described in [16] one can derive a new procedure based on the soft-thresholded BLUE.

3. Comparison between the LASSO estimator and the soft-thresholded BLUE

When we want to recover the non-null components of β^* , the soft-thresholded BLUE outperforms the LASSO estimator, solution of (2), as evidenced hereafter.

3.1. Support recovery

Let ε be a Gaussian vector of \mathbb{R}^2 having a $\mathcal{N}(0, Id_2)$ distribution, let $\beta^* = (t, 0) \in \mathbb{R}^2$ with $t \neq 0$, let X be the design matrix described hereafter and let $Y = X\beta^* + \varepsilon$.

$$X = \begin{pmatrix} 1/2 & 1/2 & 1/2 & 1/2 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}' \text{ and thus } \hat{\beta}^{\text{blue}} \sim \mathcal{N} \left(\begin{pmatrix} t \\ 0 \end{pmatrix}, \begin{pmatrix} 5 & -2 \\ -2 & 1 \end{pmatrix} \right).$$

When $u \in \mathbb{R}^p$, let us set $\text{supp}(u) := \{i \in \{1, \dots, p\} \mid u_i \neq 0\}$. Now let us denote respectively $\hat{\beta}^{\text{lasso}}(\lambda)$ and $\hat{\beta}^s(\lambda)$ the LASSO estimator and the soft-thresholded BLUE to stress that these estimators depend on λ . Whatever $\lambda > 0$, and even if $|t|$ is infinitely large, the following inequality [18,19] holds

$$\mathbb{P} \left(\text{supp}(\hat{\beta}^{\text{lasso}}(\lambda)) = \text{supp}(\beta^*) \right) \leq 1/2.$$

This inequality is illustrated in Figure 2 when $\lambda \in \{1/2, 1\}$.

On the other hand, if we take $s_1 = \sqrt{5}, s_2 = 1$ and λ as the $1 - \alpha$ quantile of a $\mathcal{N}(0, 1)$ distribution in (5), we have $\mathbb{P}(\text{supp}(\hat{\beta}^s(\lambda)) = \text{supp}(\beta^*)) \approx 1 - \alpha$ when $|t|$ is large. Consequently, by using the soft-thresholded BLUE, the probability to recover $\text{supp}(\beta^*)$ can be arbitrarily close to 1 when holds: $|t|$ is large and α is small.

3.2. Estimation of β^*

When the covariance matrix Γ is not a scalar matrix then, usually, the LASSO estimator is computed after whitening the noise as follows:

$$\hat{\beta}^{\text{lasso,w}}(\lambda) := \underset{\beta \in \mathbb{R}^p}{\text{argmin}} \left\{ \frac{1}{2} \left\| \Gamma^{-1/2}Y - \Gamma^{-1/2}X\beta \right\|^2 + \lambda \|\beta\|_1 \right\}. \quad (7)$$

When $\lambda = 0$ the above estimator coincides with the BLUE and thus has a smaller L_2 risk than the LASSO estimator as computed in (2) which is equal to the OLS estimator. The estimator given in (8) also coincides with the BLUE when $\lambda = 0$. Let $s := (s_1, \dots, s_p)$ where s_1, \dots, s_p are standard errors of the BLUE (thus s_1^2, \dots, s_p^2 are the diagonal components of $(X'\Gamma^{-1}X)^{-1}$). The soft-thresholded BLUE is defined as

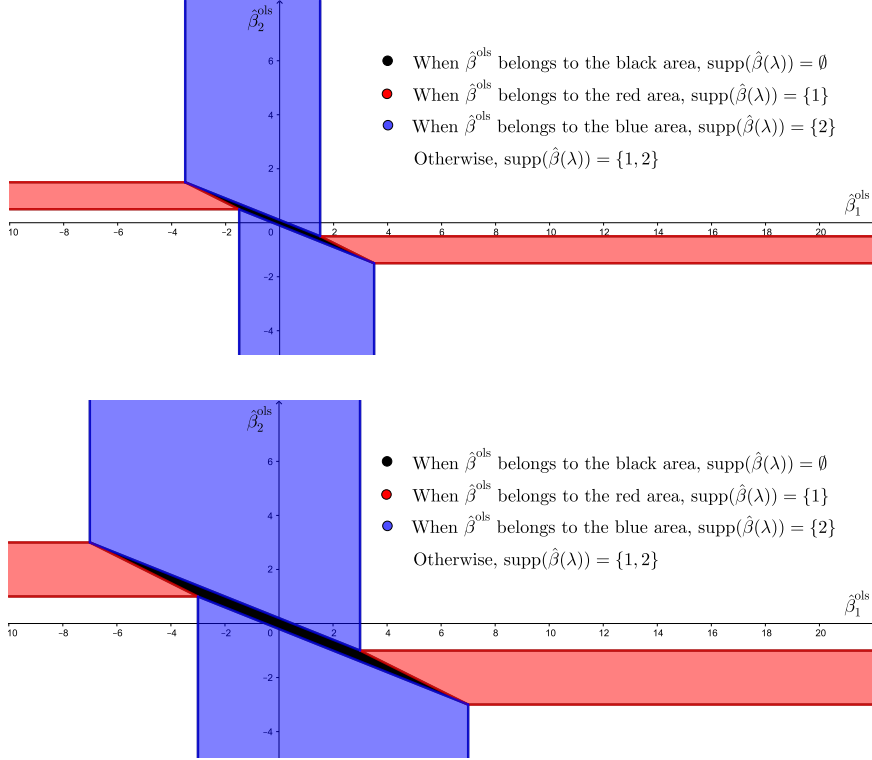


Figure 2. These figures provide the relationship between $\hat{\beta}^{\text{ols}}$ and the set of non-null components of the LASSO estimator $\text{supp}(\hat{\beta}^{\text{lasso}}(\lambda))$ (as explained in [20]) when $\lambda = 0.5$ (above) and $\lambda = 1$ (below). The x-axis and y-axis represent respectively the first and second component of the OLS estimator. One may notice that the estimator $\text{supp}(\hat{\beta}^{\text{lasso}}(\lambda))$ recovers the true set $\{1\}$ when $\hat{\beta}^{\text{ols}}$ is in the red area. Because $\hat{\beta}^{\text{ols}}$ is in the red area, this implies that $\beta_1^{\text{ols}}\beta_2^{\text{ols}} \leq 0$, and because $\mathbb{P}(\beta_1^{\text{ols}}\beta_2^{\text{ols}} \leq 0) \leq 1/2$, one may deduce that $\mathbb{P}(\text{supp}(\hat{\beta}^{\text{lasso}}(\lambda)) = \{1\}) \leq 1/2$.

follows

$$\begin{aligned}
 \tilde{\beta}^s(\lambda) &:= \underset{\beta \in \mathbb{R}^p}{\text{argmin}} \left\{ \frac{1}{2} \|U_s Y - U_s X \beta\|^2 + \lambda \|\beta\|_1 \right\} \\
 \Leftrightarrow \tilde{\beta}^s(\lambda) &= \left(\text{sign}(\hat{\beta}_i^{\text{blue}}) (|\hat{\beta}_i^{\text{blue}}| - \lambda s_i)_+ \right)_{1 \leq i \leq p}. \quad (8)
 \end{aligned}$$

Hereafter we compare estimators described in (7) and (8) with respect to the L_2 risk.

Let $Y = X\beta^* + \varepsilon$ where $X = Id_p$, $\beta^* \in \mathbb{R}^p$ and ε is a Gaussian vector in \mathbb{R}^p having a $\mathcal{N}(\mathbf{0}, \Gamma)$ distribution. The performance of the LASSO as well as the soft-thresholded BLUE depend on the design X and on Γ . By taking $X = Id_p$, we only focus on the whitening preliminary step for the LASSO. In Figure 3, we compare the following functions

$$\lambda \geq 0 \mapsto \mathbb{E}(\|\hat{\beta}^{\text{lasso,w}}(\lambda) - \beta^*\|^2) \text{ and } \lambda \geq 0 \mapsto \mathbb{E}(\|\tilde{\beta}^s(\lambda) - \beta^*\|^2).$$

in the particular settings described hereafter:

- **Equicorrelated case:** Let Γ be a 10×10 matrix whose diagonal and non-diagonal coefficients are respectively equal to 1 and c where $c \in \{0.3, 0.9\}$ and let $\beta^* = (1, \dots, 1) \in \mathbb{R}^{10}$ so that $\|\beta^*\|^2 = \mathbb{E}(\|Y - \beta^*\|^2)$.
- **Correlation exponentially decreasing:** Let Γ be a 10×10 matrix where $\Gamma_{ij} = c^{|i-j|}$ for $1 \leq i, j \leq 10$ and $c \in \{0.7, 0.9\}$ and let $\beta^* = (1, \dots, 1) \in \mathbb{R}^{10}$.

Figure 3 illustrates that, when the tuning parameter is appropriately selected for both $\hat{\beta}^{\text{lasso,w}}$ and $\hat{\beta}^s$, the L_2 risk of the soft-thresholded BLUE is approximately equal or smaller than the L_2 risk of the LASSO estimator.

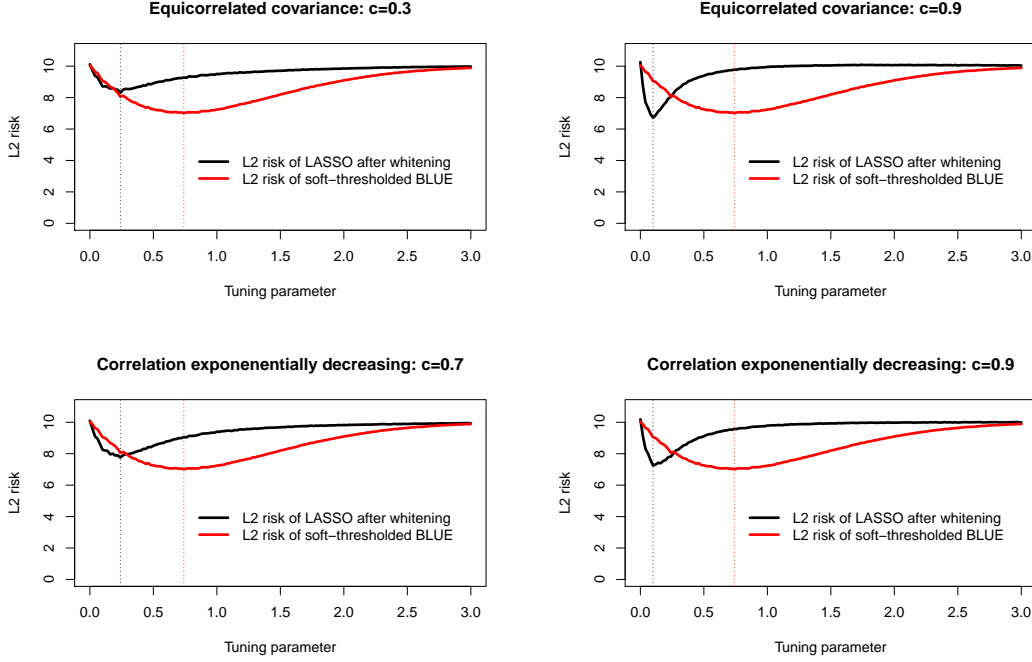


Figure 3. The x-axis and y-axis of these curves represent respectively the tuning parameter $\lambda \geq 0$ and the L_2 risk for both LASSO and soft-thresholded BLUE estimators. To obtain these curves we simulated 10000 the random vector Y and we computed the soft thresholded BLUE and LASSO estimator for $\lambda \in \{0, 0.02, 0.04, \dots, 3\}$. Computation of the LASSO estimator have been done with glmnet package [21]. In every cases, when $\lambda = 0$ these two functions are equal to $\mathbb{E}(\|Y - \beta^*\|^2)$ and when λ is very large these two functions are approximately equal to $\|\beta^*\|_2^2$. One can notice that the function $\lambda \geq 0 \mapsto \mathbb{E}(\|\hat{\beta}^s(\lambda) - \beta^*\|^2)$ does not change in these four settings since, in each case, components of the BLUE have a $\mathcal{N}(1, 1)$ marginal distribution. The minimum is 7.01 and is reached at $\lambda = 0.74$. Depending on the setting, the minimum of the function $\lambda \geq 0 \mapsto \mathbb{E}(\|\hat{\beta}^{\text{lasso,w}}(\lambda) - \beta^*\|^2)$ is 8.30, 6.71, 7.76 and 7.25 is reached at $\lambda = 0.24, \lambda = 0.10, \lambda = 0.24$ and $\lambda = 0.10$. Overall, after choosing properly the tuning parameter, one may notice that the L_2 risk is approximately equal or slightly smaller for the soft-thresholded BLUE than for the LASSO estimator.

4. Conclusion

Up to a transformation, the LASSO and the SLOPE have simple and explicit writing. In addition, our results point out that methods using the LASSO or the SLOPE in low-dimension can be derived as methods which only use the BLUE. Then, comparisons with the LASSO estimator showed the benefits of the soft-thresholded BLUE.

Acknowledgements

Patrick Tardivel thanks Professor Bogdan to allow him to continue his research at the Mathematics Institute of Wrocław University. Authors thank Artur Bogdan for his careful reading.

Disclosure statement

No potential conflict of interest was reported by the authors.

Funding

This work is part of the project GMO90+ supported by the grant CHORUS 2101240982 from the Ministry of Ecology, Sustainable Development and Energy in the national research program RiskOGM. Patrick Tardivel is partly supported by a PhD fellowship from GMO90+. We also received a grant for the project from the IDEX of Toulouse ‘Transversalité 2014’.

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Appendix A. Proof of the theorem 2.1

Sketch of proof

Theorem 2.1 is a straightforward consequence of proposition A.1. Our goal is thus to prove this proposition, which provides an explicit expression for the minimizer of $x \in \mathbb{R}^p \mapsto \frac{1}{2}\|y - x\|^2 + J(x)$ (where $y \in \mathbb{R}^p$ is a fixed vector such that $y_1 \geq y_2 \geq \dots \geq y_p \geq 0$).

Looking at the output of the algorithm described in [2] allowed us to conjecture the following two minor results:

- 1) The null vector is the unique minimizer of $x \in \mathbb{R}^p \mapsto \frac{1}{2}\|y - x\|^2 + J(x)$ when $(S_k)_{1 \leq k \leq p}$ is negative.
- 2) The vector $(S_p/p, \dots, S_p/p)$ is the unique minimizer of $x \in \mathbb{R}^p \mapsto \frac{1}{2}\|y - x\|^2 + J(x)$ when the Cesàro sequence $(S_k/k)_{1 \leq k \leq p}$ reaches its maximum at $k = p$ and when $S_p > 0$.

Statements 1) and 2) are proved respectively in lemma A.3 and in lemma A.4. These two lemmas are the keystones of the proof of proposition A.1.

In these lemmas we need to prove that an element u belongs to a closed convex set C . To prove this belonging, we use the fact that C is the intersection of all half-spaces that contain it (see [22] page 49). Consequently, if $a_1x_1 + \dots + a_px_p \geq b$ is an arbitrary half-space containing C then, to show that $u \in C$, it is enough to prove that $a_1u_1 + \dots + a_pu_p \geq b$.

Let $v \in \mathbb{R}^p$, let $[\cdot]$ be a permutation so that $|v_{[1]}| \geq \dots \geq |v_{[p]}|$, and let r be an arbitrary permutation of $\{1, \dots, p\}$. One of the key inequalities in lemma A.2 is the following one

$$\lambda_1|v_{[1]}| + \dots + \lambda_p|v_{[p]}| \geq \lambda_{r(1)}|v_1| + \dots + \lambda_{r(p)}|v_p|, \text{ where } \lambda_1 \geq \dots \geq \lambda_p > 0.$$

Proof of the proposition A.1

First, let us notice that when X is orthogonal the following equivalence holds

$$\hat{\beta}^{\text{slope}} := \operatorname{argmin}_{\beta \in \mathbb{R}^p} \frac{1}{2} \|Y - X\beta\|^2 + J(\beta) \Leftrightarrow \hat{\beta}^{\text{slope}} := \operatorname{argmin}_{\beta \in \mathbb{R}^p} \frac{1}{2} \|\hat{\beta}^{\text{ols}} - \beta\|^2 + J(\beta).$$

Consequently, to prove theorem 2.1, one only needs to provide an explicit expression of the minimizer of the function ϕ defined hereafter

$$\forall x \in \mathbb{R}^p, \phi(x) = \frac{1}{2} \|y - x\|^2 + J(x), \text{ where } y \in \mathbb{R}^p \text{ is a fixed vector.}$$

Let us notice that ϕ is a coercive and strictly convex function, thus whatever $y \in \mathbb{R}^p$, ϕ has a unique minimizer. As suggested by assumption 2.1 in the article of [2], one can restrict the study of the function ϕ to $y_1 \geq y_2 \geq \dots \geq y_p \geq 0$. Actually finding the minimizer in this particular case makes it possible to recover easily the minimizer of ϕ when y is an arbitrary vector of \mathbb{R}^p as explained in [2]. Let us remind some basic notions of sub-differentiability. Let $\epsilon > 0$, let $f : \mathbb{R}^p \rightarrow \mathbb{R}$ be a convex function, the sub-differential of f at the point $x \in \mathbb{R}^p$ denoted $\partial f(x)$ is the convex set described hereafter.

$$\begin{aligned} s \in \partial f(x) & \text{ if } \forall h \in B(0, \epsilon), f(x+h) - f(x) \geq \langle s, h \rangle \\ \Leftrightarrow s \in \partial f(x) & \text{ if } \forall h \in \mathbb{R}^p, f(x+h) - f(x) \geq \langle s, h \rangle. \end{aligned}$$

The sub-differentiability makes it possible to characterise the minimizer of ϕ (see *e.g* [23] page 177). The point x^* is a minimizer of ϕ if and only if $\mathbf{0} \in \partial \phi(x^*)$.

Proposition A.1. *Let $\phi : x \in \mathbb{R}^p \mapsto \frac{1}{2} \|y - x\|^2 + J(x)$ with $y_1 \geq \dots \geq y_p \geq 0$, let $(S_k)_{1 \leq k \leq p}$ be a sequence such that $S_k = \sum_{i=1}^k y_i - \lambda_i$ and let $1 \leq k_1 \leq \dots \leq k_s = p$ be a partition of $\{1, \dots, p\}$ such that*

$$k_1 = \max \left\{ \operatorname{argmax}_{k \in \{1, \dots, p\}} \left\{ \frac{S_k}{k} \right\} \right\} \text{ and } \forall i \in \{2, \dots, s\}, k_i = \max \left\{ \operatorname{argmax}_{k > k_{i-1}} \left\{ \frac{S_k - S_{k_{i-1}}}{k - k_{i-1}} \right\} \right\}.$$

Let $c_1 = S_{k_1}/k_1$ and for all $i \in \{2, \dots, s\}$, $c_i = (S_{k_i} - S_{k_{i-1}})/(k_i - k_{i-1})$ and let $x^ \in \mathbb{R}^p$ be a vector such that*

$$x^* = \underbrace{((c_1)_+, \dots, (c_1)_+)}_{k_1 \text{ components}}, \underbrace{(c_2)_+, \dots, (c_2)_+}_{k_2 - k_1 \text{ components}}, \dots, \underbrace{(c_s)_+, \dots, (c_s)_+}_{k_s - k_{s-1} \text{ components}}.$$

Then the unique minimizer of ϕ is x^ .*

Hereafter the SLOPE norm J is also denoted $J_{\lambda_1, \dots, \lambda_p}$, the set of permutations of $\{1, \dots, p\}$ is denoted \mathfrak{S}_p and given $u \in \mathbb{R}^p$, the permutation $[\cdot] \in \mathfrak{S}_p$ is such that $|u_{[1]}| \geq \dots \geq |u_{[p]}|$.

Lemma A.2. *Properties i) and ii) deal with the sub-differential of J and property iii) deals with the sub-differential of ϕ .*

i) *If $x_1 = \dots = x_p > 0$, then $\operatorname{conv}((\lambda_{r(1)}, \dots, \lambda_{r(p)})_{r \in \mathfrak{S}_p}) \subset \partial J(x)$.*

- ii) If $x = \mathbf{0}$, then $\text{conv} \left(\bigcup_{r \in \mathfrak{S}_p} [-\lambda_{r(1)}, \lambda_{r(1)}] \times \cdots \times [-\lambda_{r(p)}, \lambda_{r(p)}] \right) \subset \partial J(x)$.
iii) Let $0 = k_0 \leq k_1 \leq \cdots \leq k_s \leq k_{s+1} = p$ be a partition of $\{1, \dots, p\}$ such that

$$x_{k_0+1} = \cdots = x_{k_1} > x_{k_1+1} = \cdots = x_{k_2} > \cdots > x_{k_{s-1}+1} = \cdots = x_{k_s} \\ > x_{k_s+1} = \cdots = x_{k_{s+1}} = 0.$$

Let $j \in \{0, \dots, s\}$ and let us define functions $\phi_1, \dots, \phi_{s+1}$ as follows

$$\phi_{j+1}(x_{k_j+1}, \dots, x_{k_{j+1}}) = \frac{1}{2} \sum_{i=k_j+1}^{k_{j+1}} (y_i - x_i)^2 + J_{\lambda_{k_j+1}, \dots, \lambda_{k_{j+1}}}(x_{k_j+1}, \dots, x_{k_{j+1}})$$

Then the sub-differential of ϕ satisfies

$$\partial\phi_1(x_1, \dots, x_{k_1}) \times \cdots \times \partial\phi_s(x_{k_{s-1}+1}, \dots, x_{k_s}) \times \partial\phi_{s+1}(\mathbf{0}) \subset \partial\phi(x).$$

Proof: First, let us prove i). Because whatever $r \in \mathfrak{S}_p$, the two following expressions hold

$$\begin{aligned} J(x+h) &= \lambda_1|(x+h)_{[1]}| + \cdots + \lambda_p|(x+h)_{[p]}|, \\ &\geq \lambda_{r(1)}|x_1+h_1| + \cdots + \lambda_{r(p)}|x_p+h_p| \text{ and} \\ J(x) &= \lambda_{r(1)}|x_1| + \cdots + \lambda_{r(p)}|x_p|, \end{aligned}$$

one may deduce that

$$J(x+h) - J(x) \geq \lambda_{r(1)}(|x_1+h_1| - |x_1|) + \cdots + \lambda_{r(p)}(|x_p+h_p| - |x_p|) \geq \lambda_{r(1)}h_1 + \cdots + \lambda_{r(p)}h_p.$$

Consequently, whatever $r \in \mathfrak{S}_p$ we have $(\lambda_{r(1)}, \dots, \lambda_{r(p)}) \in \partial J(x)$. Furthermore, because $\partial J(x)$ is a convex set, one may deduce result i).

Now, let us prove ii), whatever $s_1 \in [-1, 1], \dots, s_p \in [-1, 1]$ whatever $r \in \mathfrak{S}_p$, the following inequality holds

$$\begin{aligned} J(h) - J(\mathbf{0}) &= \lambda_1|h_{[1]}| + \cdots + \lambda_p|h_{[p]}| \geq \lambda_{r(1)}|h_1| + \cdots + \lambda_{r(p)}|h_p| \geq \\ &\lambda_{r(1)}s_1h_1 + \cdots + \lambda_{r(p)}s_ph_p. \end{aligned}$$

Thus $[-\lambda_{r(1)}, \lambda_{r(1)}] \times \cdots \times [-\lambda_{r(p)}, \lambda_{r(p)}] \in \partial J(\mathbf{0})$. Because $\partial J(\mathbf{0})$ is a convex set, one may deduce result ii).

Finally, let us show iii). Let $h \in \mathbb{R}^p$ be small enough so that whatever $i \in \{1, \dots, s\}$, the inequality $x_{k_i} - \|h\|_\infty > x_{k_{i+1}} + \|h\|_\infty$ occurs (such a small h ensures that the k_i^{th} largest components of $x+h$ are $x_1+h_1, \dots, x_{k_i}+h_{k_i}$ and so on). As a consequence, the SLOPE norm satisfies the following equality

$$J_{\lambda_1, \dots, \lambda_p}(x+h) = \sum_{i=0}^s J_{\lambda_{k_i+1}, \dots, \lambda_{k_{i+1}}}(x_{k_i+1} + h_{k_i+1}, \dots, x_{k_{i+1}} + h_{k_{i+1}}).$$

When h is small enough, one may deduce that whatever $u \in \partial\phi_1(x_1, \dots, x_{k_1}) \times \cdots \times$

$\partial\phi_s(x_{k_{s-1}+1}, \dots, x_{k_s})$ then $u \in \partial\phi(x)$. Indeed $\phi(x+h) - \phi(x)$ is equal to

$$\begin{aligned} & \sum_{i=0}^s (\phi_{i+1}(x_{k_i+1} + h_{k_i+1}, \dots, x_{k_{i+1}} + h_{k_{i+1}}) - \phi_{i+1}(x_{k_i+1}, \dots, x_{k_{i+1}})) \\ & \geq \sum_{i=0}^s u_{k_i+1} h_{k_i+1} \times \dots \times u_{k_{i+1}} h_{k_{i+1}} = \langle u, h \rangle. \end{aligned}$$

Consequently, $u \in \partial\phi(x)$, which ensures that iii) holds. \square

Lemma A.3. *Let us assume that $\forall i \in \{1, \dots, p\}, S_i \leq 0$, then the unique minimizer of $\phi : x \in \mathbb{R}^p \mapsto \frac{1}{2}\|y - x\|^2 + J(x)$ is $x^* = (0, \dots, 0)$.*

Proof: To prove that $x^* = (0, \dots, 0)$ is a minimizer of ϕ , it suffices to show that $\mathbf{0} \in \partial\phi(x^*)$. Let us give the following equivalences

$$\mathbf{0} \in \partial\phi(x^*) \Leftrightarrow \mathbf{0} \in -y + x^* + \partial J(x^*) \Leftrightarrow y \in \partial J(\mathbf{0}).$$

By lemma 2, the sub-differential of ϕ at $\mathbf{0}$ contains the set C given hereafter

$$C := \text{conv} \left(\bigcup_{r \in \mathfrak{S}_p} [-\lambda_{r(1)}, \lambda_{r(1)}] \times \dots \times [-\lambda_{r(p)}, \lambda_{r(p)}] \right) \subset \partial J(\mathbf{0}).$$

Let us remind that a closed convex set is the intersection of all closed half-spaces containing it. Let $a_1x_1 + \dots + a_px_p \geq b$ be an arbitrary closed half-space containing C . To prove that $y \in C$, we are going to show that $a_1y_1 + \dots + a_py_p \geq b$. Let (\cdot) be a permutation of $\{1, \dots, p\}$ such that $|a_{(1)}| \leq \dots \leq |a_{(p)}|$ and let us denote $u_i = |a_{(i+1)}| - |a_{(i)}|$ with $i \in \{1, \dots, p-1\}$. Because $v := (-\lambda_p \text{sign}(a_{(1)}), \dots, -\lambda_1 \text{sign}(a_{(p)})) \in C$ and because whatever $r \in \mathfrak{S}_p$, $(v_{r(1)}, \dots, v_{r(p)}) \in C$, one may deduce that $a_{(1)}v_1 + \dots + a_{(p)}v_p = -\lambda_p|a_{(1)}| - \dots - \lambda_1|a_{(p)}| \geq b$. The following implications show that $a_1y_1 + \dots + a_py_p \geq -\lambda_p|a_{(1)}| - \dots - \lambda_1|a_{(p)}| \geq b$. We deduce from this last inequality that

$$\begin{aligned} & a_1y_1 + \dots + a_py_p \geq -\lambda_p|a_{(1)}| - \dots - \lambda_1|a_{(p)}|, \\ \Leftrightarrow & a_{(1)}y_{(1)} + \lambda_p|a_{(1)}| + \dots + a_{(p)}y_{(p)} + \lambda_1|a_{(p)}| \geq 0, \\ \Leftrightarrow & |a_{(1)}| (\text{sign}(a_{(1)})y_{(1)} + \lambda_p) + \dots + |a_{(p)}| (\text{sign}(a_{(p)})y_{(p)} + \lambda_1) \geq 0, \\ \Leftrightarrow & |a_{(1)}| \left(\sum_{i=1}^p \lambda_i + \sum_{i=1}^p \text{sign}(a_{(i)})y_{(i)} \right) + \sum_{i=1}^{p-1} u_i \left(\sum_{j=1}^{p-i} \lambda_j + \sum_{j=i}^p \text{sign}(a_{(j)})y_{(j)} \right) \geq 0. \end{aligned}$$

The last expression comes from the identity $|a_{(1)}|b_1 + \dots + |a_{(p)}|b_p = |a_{(1)}|(b_1 + \dots + b_p) + u_1(b_2 + \dots + b_p) + \dots + u_{p-1}b_p$. Finally, because $y_1 \geq \dots \geq y_p \geq 0$ one may deduce

the inequality given hereafter which ensures that $a_1y_1 + \dots + a_p y_p \geq b$. In other terms,

$$\begin{aligned}
|a_{(1)}| \left(\sum_{i=1}^p \lambda_i + \sum_{i=1}^p \text{sign}(a_{(i)})y_{(i)} \right) + \sum_{i=1}^{p-1} u_i \left(\sum_{j=1}^{p-i} \lambda_j + \sum_{j=i+1}^p \text{sign}(a_{(j)})y_{(j)} \right) \\
\geq |a_{(1)}| \left(\sum_{i=1}^p \lambda_i - \sum_{i=1}^p y_i \right) + \sum_{i=1}^{p-1} u_i \left(\sum_{j=1}^{p-i} \lambda_j - \sum_{j=1}^{p-i} y_j \right) \\
\geq -|a_{(1)}|S_p - \sum_{i=1}^{p-1} u_i S_i \geq 0.
\end{aligned}$$

Consequently, $y \in C$ and so $x^* = (0, \dots, 0)$ is the unique minimizer of ϕ . \square

Lemma A.4. *Let us assume that $\forall i \in \{1, \dots, p\}, S_i/i \leq S_p/p$ and $S_p > 0$, then the unique minimizer of $\phi : x \in \mathbb{R}^p \mapsto \frac{1}{2}\|y - x\|^2 + J(x)$ is $x^* = (S_p/p, \dots, S_p/p)$.*

Proof: To prove that x^* is a minimizer of ϕ , it suffices to show that $\mathbf{0} \in \partial\phi(x^*)$. Let us give the following equivalences

$$\mathbf{0} \in \partial\phi(x^*) \Leftrightarrow \mathbf{0} \in -y + x^* + \partial J(x^*) \Leftrightarrow y - x^* \in \partial J(x^*).$$

By the lemma A.2, $\text{conv}((\lambda_{r(1)}, \dots, \lambda_{r(p)})_{r \in \mathfrak{S}_p}) \subset \partial J(x^*)$. Hereafter we are going to show

$-y + x^* \in \text{conv}((\lambda_{r(1)}, \dots, \lambda_{r(p)})_{r \in \mathfrak{S}_p})$. Let us remind that a closed convex set is the intersection of all closed half-spaces containing it. Let $a_1x_1 + \dots + a_px_p \geq b$ be an arbitrary closed half-space containing $\text{conv}((\lambda_{r(1)}, \dots, \lambda_{r(p)})_{r \in \mathfrak{S}_p})$. To prove that $y - x^* \in \text{conv}((\lambda_{r(1)}, \dots, \lambda_{r(p)})_{r \in \mathfrak{S}_p})$, it suffices to prove that $a_1(y_1 - x_1^*) + \dots + a_p(y_p - x_p^*) \geq b$. Let (\cdot) be a permutation of $\{1, \dots, p\}$ such that $a_{(1)} \leq \dots \leq a_{(p)}$ and let us denote $u_i = a_{(i+1)} - a_{(i)}$ with $i \in \{1, \dots, p-1\}$. By definition of the half-space $a_1x_1 + \dots + a_px_p \geq b$, an appropriate permutation $r \in \mathfrak{S}_p$ ensures that $a_{(1)}\lambda_1 + \dots + a_{(p)}\lambda_p \geq b$. The following implications show that $a_1(y_1 - x_1^*) + \dots + a_p(y_p - x_p^*) \geq a_{(1)}\lambda_1 + \dots + a_{(p)}\lambda_p \geq b$.

$$\begin{aligned}
& a_1(y_1 - x_1^*) + \dots + a_p(y_p - x_p^*) \geq a_{(1)}\lambda_1 + \dots + a_{(p)}\lambda_p, \\
\Leftrightarrow & a_{(1)} \left(y_{(1)} - \frac{S_p}{p} - \lambda_1 \right) + \dots + a_{(p)} \left(y_{(p)} - \frac{S_p}{p} - \lambda_p \right) \geq 0, \\
\Leftrightarrow & a_{(1)} \underbrace{\left(\sum_{i=1}^p y_{(i)} - S_p - \sum_{i=1}^p \lambda_i \right)}_{=0} + \sum_{i=1}^{p-1} u_i \left(\sum_{j=i+1}^p y_{(j)} - (p-i)\frac{S_p}{p} - \sum_{j=i+1}^p \lambda_j \right) \geq 0.
\end{aligned}$$

The last expression comes from the identity $a_{(1)}b_1 + \dots + a_{(p)}b_p = a_{(1)}(b_1 + \dots + b_p) + u_1(b_2 + \dots + b_p) + \dots + u_{p-1}b_p$. Finally, because $y_1 \geq \dots \geq y_p \geq 0$ and because whatever $i \in \{1, \dots, p\}, S_i/i \leq S_p/p$ one may deduce the inequalities given hereafter

which ensures that $a_1(-y_1 + x_1^*) + \dots + a_p(-y_p + x_p^*) \geq b$.

$$\begin{aligned} \sum_{i=1}^{p-1} u_i \left(\sum_{j=i+1}^p y_{(j)} - (p-i) \frac{S_p}{p} - \sum_{j=i+1}^p \lambda_j \right) &\geq \sum_{i=1}^{p-1} u_i \left(\sum_{j=i+1}^p (y_j - \lambda_j) - (p-i) \frac{S_p}{p} \right), \\ &\geq \sum_{i=1}^{p-1} u_i \left(S_p - S_i - (p-i) \frac{S_p}{p} \right), \\ &\geq \sum_{i=1}^{p-1} i u_i \left(\frac{S_p}{p} - \frac{S_i}{i} \right) \geq 0. \end{aligned}$$

Consequently, $-y + x^* \in \text{conv}((\lambda_{r(1)}, \dots, \lambda_{r(p)})_{r \in \mathfrak{S}_p})$ thus $x^* = (S_p/p, \dots, S_p/p)$ is the unique minimizer of ϕ . \square

Proof of the proposition A.1: First, let us show that $c_1 > c_2 > \dots > c_s$. By construction $c_1 \geq c_2 \geq \dots \geq c_s$, thus let us show that whatever $i \in \{1, \dots, s-1\}$, the inequality $c_{i+1} = c_i$ cannot occur. Indeed, the following equality always holds

$$\frac{S_{k_{i+1}} - S_{k_{i-1}}}{k_{i+1} - k_{i-1}} = c_{i+1} \frac{k_{i+1} - k_i}{k_{i+1} - k_{i-1}} + c_i \frac{k_i - k_{i-1}}{k_{i+1} - k_{i-1}} \quad (\text{by setting } k_0 = 0 \text{ and } S_{k_0} = 0).$$

Consequently, if $c_{i+1} = c_i$ one may deduce that $k_{i+1} \in \text{argmax}_{k > k_{i-1}} \left\{ \frac{S_k - S_{k_{i-1}}}{k - k_{i-1}} \right\}$. Because $k_{i+1} > k_i$, this contradicts k_i being the largest element of $\text{argmax}_{k > k_{i-1}} \left\{ \frac{S_k - S_{k_{i-1}}}{k - k_{i-1}} \right\}$.

First, let us assume that $c_1 > \dots > c_s > 0$, then the lemma A.2 ensures that

$$\partial\phi(x^*) = \underbrace{\partial\phi_1(c_1, \dots, c_1)}_{k_1 \text{ components}} \times \dots \times \underbrace{\partial\phi_s(c_s, \dots, c_s)}_{k_s - k_{s-1} \text{ components}}.$$

Lemma A.4 ensures that whatever $i \in \{1, \dots, s\}$, we have $\mathbf{0} \in \partial\phi_i(c_i, \dots, c_i)$. Thus $\mathbf{0} \in \partial\phi(x^*)$, which ensures that x^* is a minimizer of ϕ .

Now, if $0 \geq c_1 > \dots > c_s$ then the sequence $(S_i)_{1 \leq i \leq p}$ is negative, thus lemma A.3 ensures that $x^* = (0, \dots, 0)$ is a minimizer of ϕ .

Finally, if $c_1 > \dots > c_{i_0} > 0 \geq c_{i_0+1} > \dots > c_s$ with $i_0 \in \{1, \dots, s-1\}$, then lemma A.2 ensures that

$$\partial\phi(x^*) = \underbrace{\partial\phi_1(c_1, \dots, c_1)}_{k_1 \text{ components}} \times \dots \times \underbrace{\partial\phi_{i_0}(c_{i_0}, \dots, c_{i_0})}_{k_{i_0} - k_{i_0-1} \text{ components}} \partial \times \phi_{i_0+1}(\mathbf{0}),$$

with ϕ_{i_0+1} as in lemma A.2. Lemma A.4 ensures that whatever $i \in \{1, \dots, i_0\}$, we have $\mathbf{0} \in \partial\phi_i(c_i, \dots, c_i)$. Furthermore, because $\forall i > k_{i_0}, (S_i - S_{k_{i_0}}) \leq 0$, lemma A.3 ensures that $\mathbf{0} \in \partial\phi_{i_0+1}(\mathbf{0})$. Thus $\mathbf{0} \in \partial\phi(x^*)$, which ensures that x^* is a minimizer of ϕ . \square