THE GEOMETRY OF PLS SHRINKAGES

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The geometrical structure of PLS shrinkages is here considered. Firstly, an explicit formula for the shrinkage vector is provided. In that expression, shrinkage factors are expressed a averages of a set of basic shrinkages that depend only on the data matrix. On the other hand, the weights of that average are multilinear functions of the observed responses. That representation allows to characterise the set of possible shrinkages and identify extreme situations where the PLS estimator has an highly nonlinear behaviour. In these situations, recently proposed measures for the degrees of freedom (DoF), that directly depend on the shrinkages, fail to provide reasonable values. It is also shown that the longstanding conjecture that the DoFs of PLS always exceeds the number PLS directions does not hold.

1. Introduction. In the last decades, the Partial Least Squares (PLS) methodology has gained high popularity among data analysts and statisticians. That approach has been applied to several statistical and data analysis problems, ranging from univariate regressions to more complex models involving multivariate responses, latent variables or functional data, to cite a few. Nonetheless, even for its simplest application, namely PLS regressions, only few fundamental results have been obtained. For instance, apart for an asymptotic approximation derived by means of a delta method (see [5, 23]), the distribution or the moments of PLS estimator are still unknown. The difficulty on tackling this task is testified by small amount of work that has been published on the top journals of methodological statistics [1, 2, 3, 4, 10, 11, 12, 17, 21, 24]. It worth adding that, a part of this set of these papers deals with extensions of the PLS approach, for instance to infinite dimensional spaces, instead of investigating the mathematical and inferential structure [4, 12, 24].

In parallel to statisticians, the numerical linear algebra community have studied the same kind of tools calling them Krylov or Conjugate Gradient methods (see [18]). Their main concern was the design of computationally efficient algorithms and the study of numerical stability properties,

MSC 2010 subject classifications: 62G05

Keywords and phrases: partial least squares, regressions, shrinkage factors, Krylov subspaces, Krylov methods, Degrees of Freedom

which often are not too good for these methods. Only about a decade ago, these two research streams have been bridged (see [8, 22]). The work here proposed takes inspiration from a paper which, firstly in that community, recognised that the data matrix does not completely defines the properties of the estimator, the final word is left to the observation vector [13]. Interestingly, despite the deep technical knowledge of these family of methods, to the knowledge of the author, the numerical linear algebra community have not yet recognised the key role played by the so called shrinkage factors [1, 10, 11, 14, 19, 16].

The analysis proposed in this paper grounds on the results available on the PLS shrinkages and tries to make a step forward in the understanding of the inner structure of the PLS regression estimators. Firstly, a novel expression for the vector of shrinkages which is explicit in terms of the observations is derived. A similar expression was proposed in [1], but only for a couple of special cases, and an analogous formula, but involving Ritz values, was derived in [19]. The latter, however, is not fully explicit, being these Ritz values only implicitly defined in terms of the observation vector.

By means of that expression the geometry of PLS shrinkage is formally characterised. The range of all possible values for the shrinkage vector is provided. This analysis encompass the one presented in [1] where shrinkage and expansion patterns were considered. It allows also to complete the work of Lingjærde and Christophersen in [19], where extreme expansion or shrinkage behaviours are studied. In their concluding table, Lingjærde and Christophersen were not able to establish bounds for one of the four extreme cases considered. Sometimes, it is also presumed that shrinkage factors cannot be negative For instance, this eventuality was not taken into account in the analysis of Butler and Denham (see [1] page 588), even though it was previously considered in [10] (see also [16]). The same oversight was made in the conclusions of [19], where the authors presumed that it was sufficient to bound shrinkages to one to avoid a "harmful" expansion. Here, it is shown, by an example, that large expansions along principal directions arise even when the observation vector is not orthogonal to those directions.

The possibility to have very large expansions, which is essentially due the highly nonlinear nature of the estimator, has serious consequences on the so-called Generalised Degrees of Freedom (GDoF), a statistic proposed as an extension of the DoF concept to nonlinear estimators [26, 7]. That statistic was later applied to PLS regressions in [17], where a conjecture, originally formulated in [10, 20] that states that the DoF of PLS are always larger than the number of PLS directions, is supported. That statement was formally proven for the single direction case and experimentally verified for the

general case. According to Kramer and Sugiyama, their tests "confirmed" that conjecture [17]. It is worth noting that that their experiments failed to support that conjecture for large models, but the authors ascribed these negative performances to numerical rounding errors. Alternative measures for the DoF of PLS parameter estimators have also been proposed in [5, 23, 25]. These statistics, however, seems to have even worse performances that the GDoF one.

Before concluding this short literature review, it should also mentioned that an interesting alternative approach for the analysis of PLS is proposed in [6], where the shrinkage properties are studied along directions that differ from the principal ones.

This paper is structured as follows. Firstly, in the next section, the PLS regression estimator is formulated as restricted least squares estimator on a Krylov supspace. After a rotation on the principal axes, the Krylov matrix is factorised as a diagonal by Vandermonde matrix product. This decomposition allows to separate the effects of the response vector from those of the singular values of the data matrix. In that section the main results are presented. In particular, a novel explicit expression where the shrinkage vector is characterised as an average of a set of "extreme" shrinkages that do not depend on the observations is provided. This expression allows to geometrically characterise the set of possible shrinkages in terms of these extreme points. The third section contains formal proofs of these results and a precise description and derivation of that geometrical structure. Finally the fourth section contains some examples and a discussion on the obtained results. These examples will show that an odd behaviour can be expected from PLS even in non extreme setups. Furthermore, a sufficient condition and counterexamples that invalidates the above mentioned conjecture on the DoF of PLS regression are presented.

2. Shrinkages for PLS regressions. Consider the estimation by means of Partial Least Squares regressions of the following linear model

$$\tilde{y} = X\tilde{\beta} + \varepsilon,$$
 $\varepsilon \sim (0, \sigma^2 I).$

where $X \in \mathbb{R}^{N \times m}$ is the regressor matrix, $\tilde{y} \in \mathbb{R}^N$ is the response vector and ε the disturbance vector [11]. Without loss of generality, the study of the partial least squares (PLS) regression can be performed by considering its projection on the principal axis of the regression matrix [1, 11, 19]. After a rotation, the normal equations associated to the above regression model

can be rewritten as

(1)
$$y = \Lambda \beta + u, \qquad u \sim (0, \sigma^2 \Lambda),$$

where Λ comes from the singular value decomposition $X = U\Lambda^{\frac{1}{2}}V^T$, $y = V^TX^T\tilde{y}$, $\beta = V^T\tilde{\beta}$ and $u = V^TX^T\varepsilon$. Here, without loss of generality, the eigenvalues λ_i $(i=1,\ldots,m)$ are assumed to be strictly positive, distinct and in decreasing order: $\lambda_1 > \lambda_2 > \cdots > \lambda_m > 0$. Hereafter, a vector of all ones is denoted by 1 and variables represented by capital letters denote diagonal matrices generated from vectors indicated by the corresponding lower-case variables, that is Y = diag(y), Z = diag(z), X = diag(z),

The PLS estimator with n < m directions is given by

$$\hat{\beta} = K(K^T \Lambda K)^{-1} K^T y,$$

where K is the $m \times n$ Krylov matrix

$$K = \begin{pmatrix} y & \Lambda y & \cdots & \Lambda^{n-1} y \end{pmatrix},$$

and it is assumed that $K^T \Lambda K$ is non-singular [1, 14, 15, 19]. The PLS prediction and the associated residuals for y are given by $\hat{y} = Py$ and r = (I - P)y with P denoting the oblique projection $P = \Lambda K(K^T \Lambda K)^{-1}K^T$.

It is convenient to factorise the Krylov matrix K as

$$(2) K = YV,$$

where V is the $m \times n$ Vandermonde matrix associated to λ given by $V = (\mathbf{1} \ \Lambda \mathbf{1} \ \cdots \ \Lambda^{n-1} \mathbf{1})$. Then, the projection matrix P can be rewritten as

$$P = Y\Lambda V(V^T Y^2 \Lambda V)^{-1} V^T Y.$$

Given the above assumptions on λ , that expression is well posed, that is $K^T \Lambda K = V^T Y^2 \Lambda V$ is non-singular, whenever y has n or more non-zero elements.

Shrinkage factors have been used in [1, 19] to study the characteristics of PLS regression parameter estimates. Shrinkages are defined as the ratios of the PLS estimated coefficients over the OLS coefficients along principal axes. Since the OLS estimator of the *i*-th coefficient is given by y_i/λ_i , the *i*-th shrinkage is given by $\omega_i = \lambda_i \hat{\beta}_i/y_i$ and the vector of shrinkages can be written as

(3)
$$\omega = Q\mathbf{1}, \qquad Q = \Lambda V(V^T \Psi \Lambda V)^{-1} V^T \Psi,$$

where $\Psi = Y^2$. Here, Q is the oblique projection on the range of ΛV along the null-space of ΨV . Note that, defining the shrinkages directly by (3) is more robust as it allows for zero elements in the response vector y. Again, for Q to be well defined, y needs to have at least n non-zero elements.

A couple of properties can be immediately drawn from (3). Firstly, the shrinkage vector ω is invariant to rescaling of the observation vector y and secondly, it does not depend on the signs the elements of y. Moreover, the shrinkage vector ω belongs to the n-dimensional linear manifold spanned by the columns of ΛV .

2.1. Main results. The task of obtaining simple and explicit expressions for the elements of the projection matrices Q and P and of the shrinkages ω is rather difficult. However, these expressions can be obtained in some special cases, for instance when the cardinality of y is exactly n, the number of PLS directions. The following results characterise the shrinkages in that case and in the general case.

Firstly, it is convenient to introduce some additional notation. The set of all subsets of S with cardinality n is denoted by $\binom{S}{n}$, the set of the first m integers is denoted by $[m] = \{1, 2, \ldots, m\}$ and [m, n] denotes the set of n-subsets of [m], that is $[m, n] = \binom{[m]}{n}$. For a set of indices $\tau \in [m, n]$ and $x \in \mathbb{R}^m$, x^{τ} and x_{τ} denote, respectively, the monomial $x^{\tau} = \prod_{i \in \tau} x_i$ and the subvector of x obtained by selecting the elements in the positions indicated by τ . The $m \times n$ selection matrix associated to that subsetting operation will be denoted by S_{τ} : $x_{\tau} = S_{\tau}^T x$. Moreover, the sets of non-negative and of positive reals will be denoted by \mathbb{R}_+ and \mathbb{R}_{++} .

Lemma 2.1. If $y = S_{\tau}y_{\tau}$ for some $\tau \subset [m, n]$ and $y_k \neq 0$ for all $k \in \tau$ then

(4)
$$\omega = \Lambda V (S_{\tau}^T \Lambda V)^{-1} \mathbf{1},$$

and

(5)
$$\omega_i = 1 - \prod_{i \in \tau} \left(1 - \frac{\lambda_i}{\lambda_j} \right), \qquad i = 1, \dots, m.$$

PROOF. Equation (4) follows from the fact that $Y = S_{\tau}S_{\tau}^{T}Y$ and that $S_{\tau}^{T}V$ is non-singular. Then, $S_{\tau}^{T}\omega = \mathbf{1}$, that is $\omega_{j} = 1$ when $j \in \tau$. Now, from (4), $1 - \omega_{i} = 1 - \sum_{k=1}^{n} \lambda_{i}^{k} \alpha_{k}$, where $\alpha_{1}, \ldots, \alpha_{n}$ are the elements of $\alpha = (S_{\tau}^{T}\Lambda V)^{-1}\mathbf{1}$. That is, $1 - \omega_{i} = p(\lambda_{i})$ is the value of a polynomial p

evaluated at λ_i . That polynomial has degree n+1 and zeros at the points λ_j , $j \in \tau$ and value 1 when evaluate at 0, that is p(0) = 1 and $p(\lambda_j) = 0$, for $j \in \tau$. The expression in (5) is a representation of that polynomial. \square

Note that, the above Lemma states that when the cardinality of y is exactly n, the shrinkage vector w depends only on the sparsity pattern of y and not on the actual values of its elements. Then, the following definition is well posed.

Definition 2.2. For $\tau \in [m, n]$, $\omega_{(\tau)}$ denotes the vector of shrinkages corresponding to $y = S_{\tau} \mathbf{1}$:

$$\omega_{(\tau)} = \Lambda V (S_{\tau}^T \Lambda V)^{-1} \mathbf{1}.$$

The following theorem states that any shrinkage vector is an average of the degenerate shrinkage vectors $\omega_{(\tau)}$, $\tau \in [m,n]$. It provides a novel representation, explicit on y, for the shrinkage vector. The proof will be given in the next section.

Theorem 2.3. If the cardinality of $\psi = Y^2 \mathbf{1}$ is at least n, then

$$\omega = \left(\sum_{\tau \in [m,n]} \psi^{\tau} \pi_{\tau}\right)^{-1} \sum_{\tau \in [m,n]} \psi^{\tau} \pi_{\tau} \omega_{(\tau)},$$

where

(6)
$$\pi_{\tau} = \lambda^{\tau} \prod_{\{j < i\} \subseteq \tau} (\lambda_i - \lambda_j)^2.$$

That is, ω is an average (a convex combination) of the extreme points $\omega_{(\tau)}$. The weights of that average, which are given by $\psi^{\tau}\pi_{\tau}$, are multilinear functions of the squared observations ψ_1, \ldots, ψ_m . An analogous expression is already known, but only for the case n = m - 1 [1].

Belonging ω to the convex hull of the set $\{\omega_{(\tau)} \mid \tau \in [m,n]\}$, extreme shrinkages will arise when y has (almost) cardinality n. Furthermore, although ω is a convex combination of the $\omega_{(\tau)}$ s, the mapping $y \to \omega$ does not range over the whole convex hull. Indeed, as it will be shown later in Section 3, the range of ω is polyhedral (an union of simplicia) and not necessarily convex.

Now, the set of possible shrinking/expanding patterns that can arise in PLS regression is characterised. Leaving y unconstrained, that set depends only on m, the number of eigenvalues and not on their actual values.

Theorem 2.4. The following relations hold for y and ω :

- a) $\omega_m < 1$ and the number of sign changes in $\omega 1$ is exactly n;
- **b)** for any signature with n sign changes ending with a negative value, there's a value of y such that $\omega 1$ has that signature.

The necessary part of Theorem 2.4 (point a) have been proven in [1]. To the author's best knowledge, the sufficient part (that is point b) is a new result. As an example Table 1 reports the list of possible signatures of $\omega - 1$ for the case m=6 and n=3. A positive sign indicates an expansion of the corresponding coefficient. A negative one corresponds to a shrinkage of the coefficient or a change in its sign, which may even be an expansion in absolute value.

Table 1 Shrinkage patterns when m=6 and n=3. Positive signs indicate expansions of the corresponding coefficient.

$sign(\omega - 1)$	Positions of sign changes
+-+	1, 2, 3
+ - + +	1, 2, 4
+ - + + + -	1, 2, 5
+ +	1, 3, 4
+ + + -	1, 3, 5
++-	1, 4, 5
+ + - +	2, 3, 4
+ + - + + -	2, 3, 5
+ + + -	2, 4, 5
+ + + - + -	3, 4, 5

3. The geometry of PLS shrinkages. To study the structure of the shrinkages it is convenient to work with the quantity $z = 1 - \omega$. That vector contains the relative residuals of PLS estimator, indeed $z = Y^{-1}(y - \Lambda \hat{\beta})$, provided that y does not have null elements. As it has already been noted on ω , z is a function of the squared observations $\Psi = Y^2$ and it does not depend on the signs of the elements of y. The object of this section is the study of the mapping

$$z: \mathcal{D} \to \mathcal{I}_z, \qquad \qquad \psi \to (I - Q(\psi))\mathbf{1},$$

where $Q(\psi) = \Lambda V (V^T \Psi \Lambda V)^{-1} V^T \Psi$, and \mathcal{D} is the subset of \mathbb{R}^m_+ whose elements have cardinality not smaller than n.

Firstly, \mathcal{I}_z , the image of z, is a subset of the affine space

(7)
$$\mathcal{A} = \mathbf{1} + \operatorname{span}(\Lambda V).$$

Next, $\omega = Q\mathbf{1}$ is the projection on span (ΛV) of $\mathbf{1}$ along the null space of ΨV . It turns out that z lies in the intersection of the null space of ΨV with the affine space \mathcal{A} . A sketch of that geometry is shown in Figure 1.

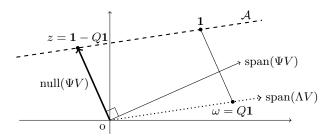


Fig 1. Geometry of the oblique projection $Q(\psi)$. The dotted and dashed lines represent, respectively, $\operatorname{span}(\Lambda V)$ and $\mathbf{1} + \operatorname{span}(\Lambda V)$. The thick segment corresponds to the vector z and the other lines to $\operatorname{span}(\Psi V)$ and $\mathbf{1} + \operatorname{null}(\Psi V)$.

Then, the couple (z, ψ) can be defined as any solution of the set of constraints

$$V^T \Psi z = 0, \qquad \qquad \psi \in \mathcal{D}, \qquad \qquad z \in \mathcal{A}.$$

Remark 3.1. The mapping z is not bijective, indeed its inverse maps $z \in \mathcal{I}_z$ to the set

$$\{\psi \in \mathcal{D} \subseteq \mathbb{R}^m_+ \mid V^T Z \psi = 0\}.$$

Note that the closure of that set is the convex cone $C_z = \{\psi \in \mathbb{R}_+^m, V^T Z \psi = 0\}$ and, thus, can be characterised by means of a finite number of extremal rays. This representation can exploited to derive the distribution density of z, or equivalently of ω , which derives by integrating the density of ψ over that set.

Another quantity that will be used in this analysis is $\alpha(\psi) = (V^T \Psi \Lambda V)^{-1} V^T \psi$. As it should have been clear, the vectors α , ω and z are now considered as functions of ψ . The mappings they define have the same domain, images that will be denoted by \mathcal{I}_{α} , \mathcal{I}_{ω} and \mathcal{I}_{z} , respectively. Note that, since $\omega(\psi)$, $z(\psi)$ and $\alpha(\psi)$ are just a linear or affine transformations of each other, most of the results derived for any of these quantities apply to the other with

only trivial modifications. Working with α will correspond to working with coordinates on the affine space \mathcal{A} , while working with z has the advantage that its signature will have a precise geometric meaning.

3.1. The shrinkage vector is an average. Consider now the behaviour of α and z on the edge of \mathcal{D} where the cardinality is exactly n. Analogously to Lemma 2.1, when $\psi = S_{\tau}\tilde{\psi}$, with $\tau \in [m, n]$ and $\tilde{\psi} \in \mathbb{R}^n_{++}$,

(8)
$$\alpha(\psi) = (S_{\tau}^T \Lambda V)^{-1} \mathbf{1},$$

and

(9)
$$z(\psi) = (I - \Lambda V (S_{\tau}^T \Lambda V)^{-1} S_{\tau}^T) \mathbf{1}.$$

From Lemma 2.1 it follows that $S_{\tau}^T \omega(\psi) = 1$ and $S_{\tau}^T z(\psi) = 0$. As already remarked, in these cases the value of α and z depends only on the sparsity pattern of ψ . The mappings $\alpha_{(\cdot)} : [m,n] \to \mathbb{R}^n$ and $z_{(\cdot)} : [m,n] \to \mathbb{R}^n$ are defined accordingly to Definition 2.2. That is, for instance,

(10)
$$\alpha_{(\cdot)}: \tau \to \alpha_{(\tau)} = \alpha(S_{\tau}\mathbf{1}) = (S_{\tau}^T \Lambda V)^{-1}\mathbf{1}.$$

The set of vectors $\{\alpha_{(\tau)}, \ \tau \in [m, n]\}$ plays a key role in the study of the image of α . Indeed, Theorem 2.3 is a corollary of the following result.

Theorem 3.2. For $\psi \in \mathcal{D}$,

$$\alpha(\psi) = \sum_{\tau \in [m,n]} p_{\tau}(\psi) \alpha_{(\tau)},$$

where
$$p_{\tau}(\psi) = \left(\sum_{s \in [m,n]} \psi^s \pi_s\right)^{-1} \psi^{\tau} \pi_{\tau}$$
, and π_{τ} is defined in (6).

PROOF. Firstly note that $\alpha = \alpha(\psi)$ solves the equation

(11)
$$V^T \Psi \Lambda V \alpha = V^T \Psi \mathbf{1}.$$

The cardinality condition on ψ is sufficient to guarantee the non-singularity of the coefficient matrix of (11). By the Kramer rule, the k-th element of α is given by

(12)
$$\alpha_k = (-1)^k \frac{\det(V^T \Psi W_{(-k)})}{\det(V^T \Psi \Lambda V)},$$

where $W_{(-k)}$ is the matrix obtained from the $m \times (n+1)$ Vandermonde matrix $(\mathbf{1} \Lambda V)$ after deleting the (k+1)-th column:

$$W_{(-k)} = \begin{pmatrix} \mathbf{1} & \Lambda \mathbf{1} & \cdots & \Lambda^{k-1} \mathbf{1} & \Lambda^{k+1} \mathbf{1} & \cdots & \Lambda^n \mathbf{1} \end{pmatrix}.$$

That is, $W_{(-k)}$ contains all the powers of λ up to n excluding the k-th one. Note that $W_{(-0)} = \Lambda V$ so that $\alpha_k = (-1)^k \det(V^T \Psi W_{(-k)}) / \det(V^T \Psi W_{(-0)})$. Now, the Cauchy-Binet formula allows to express the determinants in (12)

$$\det(V^T \Psi W_{(-k)}) = \sum_{\tau \in [m,n]} \psi^\tau \det(S_\tau^T V) \det(S_\tau^T W_{(-k)}).$$

Then, setting $\pi_{\tau} = \det(S_{\tau}^T V) \det(S_{\tau}^T W_{(-0)})$ gives

(13)
$$\alpha_k = \frac{1}{\sum_{\tau \in [m,n]} \psi^{\tau} \pi_{\tau}} \sum_{\tau \in [m,n]} \psi^{\tau} \pi_{\tau} \alpha_{(\tau),k}, \text{ with } \alpha_{(\tau),k} = (-1)^k \frac{\det(S_{\tau}^T W_{(-k)})}{\det(S_{\tau}^T W_{(-0)})}.$$

The expression (6) for π_{τ} derives by noting that, since $S_{\tau}^{T}V$ is a square Vandermonde matrix,

$$\det(S_{\tau}^T V) = \prod_{\{j < i\} \subseteq \tau} (\lambda_i - \lambda_j),$$

and

as

$$\det(S_{\tau}^T W_{(-0)}) = \det(S_{\tau}^T \Lambda V) = \lambda^{\tau} \det(S_{\tau}^T V).$$

The proof is concluded by noting that when ψ has cardinality n, the summations in (13) have only one non-zero term and, thus, $\alpha_{(\tau),k}$ defined in (13) is equal to the k-th element of the vector $\alpha_{(\tau)}$ defined in (10). Indeed,

Corollary 3.3. If $\psi \in \mathcal{D}$ then

$$\omega(\psi) = \sum_{\tau \in [m,n]} p_{\tau}(\psi)\omega_{(\tau)} \qquad and \qquad z(\psi) = \sum_{\tau \in [m,n]} p_{\tau}(\psi)z_{(\tau)}.$$

PROOF. The corollary follows directly noting that $\omega(\psi) = \Lambda V \alpha(\psi)$ and $z(\psi) = \mathbf{1} - \Lambda V \alpha(\psi)$.

Since the object of the analysis will mainly be the relative residual vector z it is convenient, for future reference, to give the explicit expression for $z_{(\tau),i}$ by rewriting (5) as

(14)
$$z_{(\tau),i} = \prod_{i \in \tau} \left(1 - \frac{\lambda_i}{\lambda_j} \right), \qquad \tau \in [m, n].$$

The marginal dependence of z on ψ_k is characterised in the following corollary.

Corollary 3.4. For $k \in [m]$, z can be written in terms of ψ_k as follows

$$z = t z|_{\psi_k=0} + (1-t)(I - \lambda_k^{-1}\Lambda)z|_{\psi=\theta}^{(n-1)}, \qquad t = \frac{1}{1 + \psi_k q_k},$$

with

$$g_k = \Big(\sum_{\tau \in \binom{[m] - \{k\}}{n}} \psi^{\tau} \pi_{\tau}\Big)^{-1} \Big(\sum_{\tau \in \binom{[m] - \{k\}}{n-1}} \psi^{\tau} \pi_{\tau \cup \{k\}}\Big),$$

and where $z|_{\psi_k=0}$ is the values of z obtained by setting $\psi_k=0$ and $z|_{\psi=\theta}^{(n-1)}$ is the value of z obtained at the previous step of the PLS method evaluated at the point $\theta=(I-\lambda_k^{-1}\Lambda)^2\psi$. Note that $\theta_k=0$.

PROOF. From (13), rewrite α as

$$z = \frac{A + C\psi_k}{B + D\psi_k} = \frac{A}{B} \cdot \frac{B}{B + D\psi_k} + \frac{C}{D} \cdot \frac{D\psi_k}{B + D\psi_k},$$

where

$$A = \sum_{\tau \in \binom{[m] - \{k\}}{n}} \psi^{\tau} \pi_{\tau} z_{(\tau)}, \qquad C = \sum_{\tau \in \binom{[m] - \{k\}}{n-1}} \psi^{\tau} \pi_{\tau \cup \{k\}} z_{(\tau \cup \{k\})},$$

$$B = \sum_{\tau \in \binom{[m] - \{k\}}{n}} \psi^{\tau} \pi_{\tau}, \qquad D = \sum_{\tau \in \binom{[m] - \{k\}}{n-1}} \psi^{\tau} \pi_{\tau \cup \{k\}}.$$

Now, write $\pi_{\tau \cup \{k\}}$ and $z_{(\tau \cup \{k\})}$ can be written in terms of π_{τ} and $z_{(\tau)}^{(n-1)}$ as follows

$$\pi_{\tau \cup \{k\}} = \prod_{j \in \tau \cup \{k\}} \lambda_j \prod_{\{j < i\} \in \tau \cup \{k\}} (\lambda_i - \lambda_j)^2 = \lambda_k \prod_{j \in \tau} (\lambda_k - \lambda_j)^2 \pi_{\tau}^{(n-1)}$$

and $z_{(\tau \cup \{k\}),p} = \prod_{j \in \tau \cup \{k\}} (1 - \lambda_j^{-1} \lambda_p) = (1 - \lambda_k^{-1} \lambda_p) z_{(\tau),p}^{(n-1)}$, that is, $z_{(\tau \cup \{k\})} = (I - \lambda_k^{-1} \Lambda) z_{(\tau)}^{(n-1)}$. Here $z_{(\tau)}^{(n-1)}$ is the value of $z_{(\tau)}$ at the step n-1. It follows that

$$\begin{split} \frac{C}{D} &= (I - \lambda_k^{-1} \Lambda) \frac{\sum_{\tau \in \binom{[m] - \{k\}}{n-1}} \psi^\tau \pi_\tau^{(n-1)} z_{(\tau)}^{(n-1)} \prod_{j \in \tau} (1 - \lambda_k^{-1} \lambda_j)^2}{\sum_{\tau \in \binom{[m] - \{k\}}{n-1}} \psi^\tau \pi_\tau^{(n-1)} \prod_{j \in \tau} (1 - \lambda_k^{-1} \lambda_j)^2} \\ &= (I - \lambda_k^{-1} \Lambda) \frac{\sum_{\tau \in \binom{[m] - \{k\}}{n-1}} \theta^\tau \pi_\tau^{(n-1)} z_{(\tau)}^{(n-1)}}{\sum_{\tau \in \binom{[m] - \{k\}}{n-1}} \theta^\tau \pi_\tau^{(n-1)}}, \end{split}$$

where $\theta_j = (1 - \lambda_k^{-1} \lambda_j)^2 \psi_j$, $j = 1, \dots, m$. The vector θ can also be written as $\theta = (I - \lambda_k^{-1} \Lambda)^2 \psi$ and then $C/D = (I - \lambda_k^{-1} \Lambda) z |_{\psi=\theta}^{(n-1)}$.

Corollary 3.4 shows that, by varying the value of ψ_k , the vector z moves along the segment with extremes $z|_{\psi_k=0}$ and $(I-\lambda_k^{-1}\Lambda)z|_{\psi=\theta}^{(n-1)}$. Those are reached when $\psi_k=0$ or $\psi_k=\infty$, respectively. That corollary gives also a representation of the shrinkages obtained at the (n-1)-th step as a limit of the ones obtained at the n-th step. That is, when ψ_k is large, the shrinkage factors can be approximated rescaling those obtained from (n-1)-steps of the PLS procedure applied to model where ψ is replaced by θ : $z=(I-\lambda_k^{-1}\Lambda)z|_{\psi=\theta}^{(n-1)}$ for large values of ψ_k . The above result allows also to derive the shrinkage or the estimator distribution conditional on $\psi_1,\ldots,\psi_{k-1},\psi_{k+1},\ldots,\psi_m$.

3.2. The shrinkage's range. Consider now the characterisation of \mathcal{I}_{α} , that is the range of the mapping α . Theorem 3.2 states that $\mathcal{I}_{\alpha} \subseteq \operatorname{conv}(\{\alpha_{\tau} \mid \tau \in [m,n]\})$, where $\operatorname{conv}(X)$ denotes the convex hull of the set X. In order to derive the actual shape of \mathcal{I}_{α} the two auxiliary results are introduced. The first one is given in the following lemma which states that the above inclusion becomes an equality, when m = n + 1.

Lemma 3.5. When m = n + 1, $\operatorname{cl}(\mathcal{I}_{\alpha}) = \operatorname{conv}(\{\alpha_{\tau}, \ \tau \in [m, n]\})$, where $\operatorname{cl}(X)$ denotes the closure of the set X.

PROOF. It need only to be proven that any element of the righthand side can be written as $\alpha(\psi)$ for some $\psi \in \mathbb{R}^m_+$. To this end, firstly note that

$$[m, n] = \{ \tau_i = [m] - \{i\}, i = 1, \dots, m \}.$$

Then, consider a generic α_* in the convex hull of $\{\alpha_{(\tau_1)}, \ldots, \alpha_{(\tau_m)}\}$:

$$\alpha_* = \sum_{i=1}^m c_i \alpha_{(\tau_i)},$$

where $c_i > 0$ and $\sum_i c_i = 1$. By Theorem 3.2, it is sufficient to find a $\psi \in \mathbb{R}_+^m$ such that $c_i = p_{\tau_i}$. To this end, note that, since $\psi^{\tau_i} = \tau_i^{-1}(\tau_1 \cdots \tau_m)$,

$$p_{\tau_i} = \frac{\psi_i^{-1} \pi_{\tau_i}}{\sum_{j=1}^m \psi_j^{-1} \pi_{\tau_j}}.$$

Then, choosing $\psi_i = \kappa \pi_{\tau_i}/c_i$, $i = 1, \ldots, m$, leads to $p_{\tau_i} = c_i$. Now, since $\pi_{\tau_i} > 0$, the elements of ψ are positive provided that $c_i > 0$. Finally, taking the closure of \mathcal{I}_{α} allows to include the remaining points of the convex hull. \square

The second result is given in the next lemma, where it is shown that any element of \mathcal{I}_{α} can be written as $\alpha(\psi)$, with the cardinality of ψ being n+1. For simplicity and without loss of generality that result is derived in term of z instead of α .

Lemma 3.6. Let $z_{\star} \in \mathcal{I}_z$, there exists $\psi \in \mathbb{R}^n$, $\psi \geq 0$, with cardinality n+1 such that $z_{\star} = z(\psi)$.

PROOF. Consider a vector $\psi_{\star} \in \mathcal{D}$ such that $z_{\star} = z(\psi)$ and $\mathbf{1}^T \psi_{\star} = 0$. Note that, by the homogeneity of z, this normalisation can be imposed without losing in generality. Now, as remarked in Section 3, such a vector should satisfy

$$V^T Z_{\star} \psi_{\star} = 0, \quad \mathbf{1}^T \psi_{\star} = 0, \quad \psi_{\star} \ge 0$$

That equation states that the origin belong to the convex-hull of the columns of $Z_{\star}V$. Then, by the Minkowski-Carathèodory theorem, it is also contained into the convex hull of a subset of this set of vectors having cardinality n+1. That is,

$$0 = V^T Z_{\star} \psi,$$
 $\psi \ge 0, \quad \mathbf{1}^T \psi = 1, \quad \operatorname{card}(\psi) = n + 1,$

which implies also that $\psi \in \mathcal{D}$ and thus $z(\psi) = z_{\star}$.

Now, a precise description of \mathcal{I}_z and, in turns of \mathcal{I}_{α} , follows directly as a corollary of Lemmata 3.5 and 3.6.

Corollary 3.7.

$$\operatorname{cl}(\mathcal{I}_z) = \bigcup_{T \in [m, n+1]} \operatorname{conv}\left(\left\{z_{(\tau)}, \ \tau \in {T \choose n}\right\}\right).$$

Note that, in general, the image of z does not correspond to the convex hull of the points $z_{(\tau)}, \ \tau \in [m,n]$. However, to characterise its geometry it is sufficient to study the relations between the tetrahedra with vertices $\{z_{(\tau)}, \tau \in {T \choose n}\}, \ T \in [m,n+1]$. The following proposition states that all the points $z_{(\tau)}$ that share a common subset τ_0 are aligned in a subspace of dimensions n-k. In particular, when k=n-1 these points are aligned (see also Corollary 3.4).

PROPOSITION 3.8. Let k < n and $\tau_0 \in [m, k]$. Then, any $z_{(\tau)}$ with $\tau \in [m, n]$ and $\tau_0 \subset \tau$ belongs to the subspace of \mathbb{R}^m

$$\mathcal{Z}_{\tau_0} = \{ z \subset \mathbb{R}^m \mid z_i = 0, \text{ for } i \in \tau_0 \}.$$

PROOF. Let S_{τ} be the selection matrix corresponding to τ . To prove this result it is sufficient to note that $S_{\tau}^T z_{(\tau)} = 0$ and that $\tau_0 \subset \tau$.

When n-k=1, besides being aligned, the points $z_{(\tau)}$, $\tau \supset \tau_0$, follow also a specific ordering. Indeed, let $\tau = \tau_0 \cup \{k\}$, by (14) the elements of $z_{(\tau)}$ can be written as $z_{(\tau),i} = (1-\lambda_i/\lambda_k) \prod_{j \in \tau_0} (1-\lambda_i/\lambda_j)$, $i=1,\ldots,n$. For example, when n=3, the points $z_{(237)}, z_{(247)}, z_{(257)}$ and $z_{(267)}$ are all

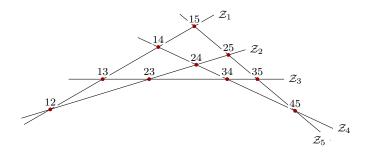


Fig 2. Geometry of $z_{(\tau)}$ for m=5, n=2. Each line represents an affine space \mathcal{Z}_i .

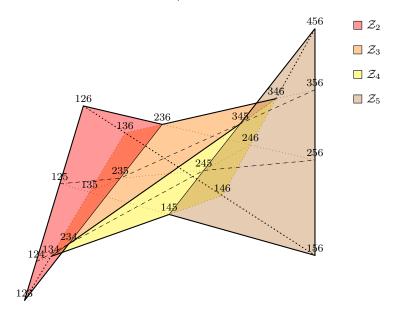


Fig 3. Geometry of $z_{(\tau)}$ for m=6, n=3 projected on the affine space \mathcal{A} . Each affine space \mathcal{Z}_i is shown in a different color except for \mathcal{Z}_1 and \mathcal{Z}_6 which are not visible here. Lines correspond to the affine spaces $\mathcal{Z}_i \cap \mathcal{Z}_j$, $i \neq j$.

aligned and ordered, in the sense that $z_{(2\underline{4}7)}$ and $z_{(2\underline{5}7)}$ belong to the segment $z_{(2\underline{3}7)}-z_{(2\underline{6}7)}$ and $z_{(2\underline{5}7)}$ to the segment $z_{(2\underline{4}7)}-z_{(2\underline{6}7)}$. It also implies that when n=3 the tetrahedron $\mathcal{T}_{1234}=\operatorname{conv}\{z_{(\tau)}\mid\tau\subset\{1,2,3,4\},\#\tau=3\}$ is contained into the tetrahedron $\mathcal{T}_{1236}=\operatorname{conv}\{z_{(\tau)}\mid\tau\subset\{1,2,3,6\},\#\tau=3\}$. Two examples of the possible configurations of $z_{(\tau)}$ are reported in Figures 2 and 3 for the cases n=2 and n=3, respectively. It should be remarked that, even though proportions changes with λ , the main features of the geometry, that is spatial alignment and ordering, remain fixed.

Each linear space \mathcal{Z}_i , $i=1,\ldots,m$, defines a partition of \mathbb{R}^m into three sets $\mathcal{Z}_i^{\pm} = \{z \mid \pm z_i > 0\}$ and \mathcal{Z}_i . Any signature of z is associated to a specific intersection of these sets. Figures 2 and 3 anticipated the geometry of the possible configurations of the points $z_{(\tau)}$, $\tau \in [m, n]$ which ultimately depends on of possible signatures of the elements of \mathcal{I}_z . This is the aspect that will be addressed in the next subsection.

3.3. The signature of z. Any subset $\tau \in [m, n]$ with cardinality n corresponds to a single point $z_{(\tau)} \in \mathcal{I}_z$. Now, consider a subset T of length n+1. That set contains n+1 subsets of length n, each one associated to a point of \mathcal{I}_z . It is not difficult to show that these points are linear independent, and

thus their convex hull is a tetrahedron or, more precisely, an n-dimensional simplex of \mathbb{R}^m . The following definition introduces the notation used to indicate that set.

Definition 3.9. For $T \in [m, n+1]$, \mathcal{T}_T denotes the n-dimensional simplex (a tetrahedron when n=3)

$$\mathcal{T}_T = \operatorname{conv}\left\{z_{(\tau)}, \mid \tau \in {T \choose n}\right\}.$$

Example 3.10. \mathcal{T}_{12357} is the simplex having vertices $z_{(2357)}$, $z_{(1357)}$, $z_{(1257)}$, $z_{(1237)}$ and $z_{(1235)}$. This simplex has n=5 faces. Each of them is defined by a n vertices and belong to one of the linear spaces $\mathcal{Z}_1, \ldots, \mathcal{Z}_5$. For instance, the corner points $z_{(1357)}$, $z_{(1257)}$, $z_{(1237)}$ and $z_{(1235)}$ identify the face which belong to \mathcal{Z}_1 . The following proposition will show that $\mathcal{T}_{12345} = (\mathcal{Z}_1^+ \cup \mathcal{Z}_2^- \cup \mathcal{Z}_3^+ \cup \mathcal{Z}_4^- \cup \mathcal{Z}_5^+) \cap \mathcal{A}$. Recall that \mathcal{A} is the n-dimensional affine space defined in (7).

Now, the signature of the elements in these simplices, $z \in \mathcal{T}_T$, is considered. It turns out that the signature at some specific positions is fixed.

PROPOSITION 3.11. Let $z \in \mathcal{T}_t$ with $t = \{t_0 < t_1 < \dots < t_n\}, t_0 > 0$ and $t_n \leq m$. Then,

$$(-1)^{n-k} z_{t_k} \ge 0,$$
 $k = 1, ..., n,$
 $z_i \ge 0,$ $i > t_n,$
 $(-1)^n z_i \ge 0,$ $i < t_0.$

PROOF. Consider the t_i -th element of a generic corner point $z_{(\tau)}$, $\tau \in {t \choose n}$. Then, $z_{(\tau),i} = 0$ if $i \in \tau$ otherwise, by (14), $(-1)^{n+1-i}z_{(\tau),i} > 0$. To conclude the proof it is sufficient to note that z is a convex combination of the corner points.

Proposition 3.12. Let
$$t = a \cup b \in [m, n+1]$$
 and $i \in [m]$. If

$$\max a < i < \min b$$
.

then \mathcal{Z}_i crosses the interior of the simplex \mathcal{T}_t . That is, there exists $z^+, z^-, z^0 \in \mathcal{T}_t$ such that $z_i^+ > 0$, $z_i^- < 0$ and $z_i^0 = 0$.

PROOF. Choose $j \in a$ and $k \in b$, and set $s = T - \{j\}$ and $t = T - \{k\}$. The *i*-th elements of $z_{(s)}$ and $z_{(t)}$ have different signs. Indeed, by (14),

$$z_{(s),i}z_{(t),i} = \prod_{h \in s} \left(1 - \frac{\lambda_i}{\lambda_j}\right) \prod_{h \in t} \left(1 - \frac{\lambda_i}{\lambda_k}\right)$$
$$= \left(1 - \frac{\lambda_i}{\lambda_j}\right) \left(1 - \frac{\lambda_i}{\lambda_k}\right) \prod_{h \in s \cap t} \left(1 - \frac{\lambda_i}{\lambda_h}\right)^2 < 0,$$

since
$$\lambda_i > \lambda_i > \lambda_k$$
.

Propositions 3.11 and 3.12 establishes a pattern for the signature of the elements of a simplex \mathcal{T}_t , $t \in [m, n+1]$. The following example gives an illustration of the above results.

Example 3.13. Let m = 12, n = 4, $t = \{2, 5, 7, 8, 10\}$. Then, the signature of the corner elements of \mathcal{T}_t and of a generic element z is reported in Table 2, where +, -, 0 and \times denote non-negative, non-positive, null and unconstrained elements.

Signatures of the vertices of $\mathcal{T}_{\{2,5,7,8,10\}}$. The last row shows the sign pattern of an internal point as prescribed by Propositions 3.11 and 3.12.

			1 1 1
	1 2 3 4	5 6 7 8 9	0 1 2
$z_{(5,7,8,10)}$	++++	0 - 0 0 -	0 + +
$z_{(2,7,8,10)}$	+ 0	$-\ -\ 0\ 0\ -$	0 + +
$z_{(2,5,8,10)}$	+ 0	0 + + 0 -	0 + +
$z_{(2,5,7,10)}$	+ 0	0 + 0	0 + +
$z_{(2,5,7,8)}$	+ 0	0 + 0 0 +	+ + +
z	$+$ + \times \times	$- \times + - \times$	+ + +

Proposition 3.12 only characterise the marginal structure of the signature of z. There is, however, a conjoint structure that links consecutive undetermined signs. The investigation of that conjoint structure is here tackled by using tools related to the concept of total positivity of matrices [9]. Before proceeding with the proof, it is necessary to introduce some definitions and results on that subject.

Definition 3.14 (Total positivity). A matrix $A \in \mathbb{R}^{m \times n}$ is totally nonnegative (positive) if the determinant of any square submatrix of A is nonnegative (positive).

Applying a totally non-negative (positive) matrix to a vector cannot increase the number of sign variations. This number is not uniquely identified when some of the elements are null and maximal/minimal quantities should be used.

Definition 3.15. Let $x \in \mathbb{R}^n$ be a vector having cardinality n (no zero elements), then v(x) denotes the number of sign changes in x:

$$v(x) = \#\{x_i x_{i+1} < 0, \ 1 < i \le n\}.$$

Definition 3.16. For $x \in \mathbb{R}^n$,

$$v_m(x) = \min\{v(y) \mid \text{card}(y) = n \text{ and } x_i y_i \ge 0, \ 1 \le i \le n\},\ v_M(x) = \max\{v(y) \mid \text{card}(y) = n \text{ and } x_i y_i \ge 0, \ 1 \le i \le n\},\$$

where $x \in \mathbb{R}^n$.

The max (min) used in Definition 3.16 is computed among the vectors y whose signature is concordant with that of the non-null part of x. That is, $v_m(x)$ counts the number of sign changes once the null elements have been removed from x. Let \bar{x} be obtained from x, by replacing the zero elements with signed values, then $v(\bar{x}) \in [v_m(x), v_M(x)]$. Then, the definition of v(x) could be extended to the mapping $x \to [v_m(x), v_M(x)] \cap \mathbb{N}$.

These measures of sign changes satisfy the property

$$v_m(x) \le v_M(x) \le n - 1,$$
 $x \in \mathbb{R}^n.$

As stated above, totally non-negative (positive) matrices do not increase the number of sign changes when applied to a vector. That fact is more precisely stated in the following Theorem.

Theorem 3.17. Let $A: m \times n$ and $x \in \mathbb{R}^n$. If A is totally non-negative then $v_m(Ax) \leq v_m(x)$. If A is totally positive and $x \neq 0$, then

$$v_M(Ax) \le v_m(x)$$
.

PROOF. See Theorems 4.2.2 and 4.3.5 in [9].

It is possible now, to establish the number of sign variations of a generic $z \in \mathcal{Z}$. The following Lemma and Corollary complete the characterisation given in Propositions 3.11 and 3.12.

Table 3

Signatures of the elements of $\mathcal{T}_{\{2,5,7,8,10\}}$. The first column contains the positions of sign changes and the first row shows the pattern prescribed by Propositions 3.11 and 3.12.

Pos.	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-
	+ + × × $-$ × + $-$ × + + $+$	F
5, 7, 8, 10 4, 7, 8, 10 3, 7, 8, 10	+ +	+
5, 6, 8, 10 4, 6, 8, 10 3, 6, 8, 10	+++++-++	+
5, 6, 8, 9 4, 6, 8, 9 3, 6, 8, 9	+++++++++++++++++++++++++++++++++++++	+ +
5, 7, 8, 9 4, 7, 8, 9 3, 7, 8, 9	+++-+++++++++++++++++++++++++++++++++++	+

Lemma 3.18. Assume that n < m. Then,

$$(15) v_M(z) \le n.$$

If $card(\psi) > n$, then

$$(16) v_m(z) \in \{n-1, n\}.$$

and $v_m(z) = n$ when $card(\psi) > n$, $z_1 \neq 0$ and $z_m \neq 0$.

Corollary 3.19. Assuming n < m, if card(z) = m then v(z) = n, $z_m > 0$ and $(-1)^n z_1 > 0$.

Before going to the proof of the Lemma, an example of its application to the characterisation of the signatures of the elements of \mathcal{T}_t is given.

Example 3.20 (Continuation of Example 3.13). The above corollary allows to identify the signature of elements of $\mathcal{T}_{\{2,5,7,8,10\}}$. For example, the uncertainty at the positions 3 and 4 corresponds to only one change of sign that can occur before the 3rd, 4th or 5th position. The possible signatures are reported in Table 3.

The following two results are instrumental to the proof of Lemma 3.18.

Lemma 3.21. The Vandermonde matrices V and ΛV are totally positive.

PROOF. It is a consequence of the ordering assumed for λ (see the introductory chapter of [9]).

PROPOSITION 3.22. Let $\Psi \in \mathcal{D}$, if $\Psi z(\psi) = 0$ then $\operatorname{card}(\psi) = n$.

PROOF. Firstly note that, since $z = \mathbf{1} - \Lambda V \alpha$ and ΛV has full column rank, the vector z cannot have more than n zero elements. Besides, \mathcal{D} does not contains vectors with more than n non-zero elements.

PROOF OF LEMMA 3.18. The first inequality (15) follows from Theorem 3.17 from the fact that $z = \mathbf{1} - \Lambda V \alpha$ and that the matrix (1 ΛV) is totally positive. For that reason, then,

(17)
$$v_M(z) \le v_m(\begin{pmatrix} 1 & -\alpha^T \end{pmatrix}) \le n.$$

Next, assuming $\operatorname{card}(\psi) > n$, Proposition 3.22 implies that $\Psi z \neq 0$ and from Theorem 3.17 it follows that

(18)
$$v_m(z) \ge v_m(\Psi z) \ge v_M(V^T \Psi z) = v_M(0) = n - 1.$$

Then, combining (17) and (18) gives (16). To show the last statement it is sufficient to note that, by Proposition 3.11, $z_m \ge 0$ and $(-1)^n z_1 \ge 0$ and that, when these elements are non-null, the minimal number of sign changes cannot be n-1.

3.4. The inverse mapping. Until now, only the image \mathcal{I}_{ω} of the mapping $\psi \to \omega$ has been considered. However, knowing the inverse mapping $\omega \to \psi$ is more helpful if one is concerned with the distribution of ω given that of ψ . In this subsection, the level sets of that function, which is not bijective, are geometrically characterised. Here, to keep the exposition short, not all the details will be formally proven.

Consider the inverse of the function $z: \psi \to z(\psi)$, which consists on the level sets $z^{-1}(\hat{z}) = \{\psi \in \mathbb{R}^m_+ \mid z(\psi) = \hat{z}\}$, with $\hat{z} \in \mathcal{I}_z$. As discussed in Remark 3.1, the closure of the inverse of z maps each value of z to the convex cone

$$\mathcal{C}_z = \{ \psi \in \mathbb{R}_+^m \mid V^T Z \psi = 0 \}.$$

Being the intersection of m half-spaces and n linear spaces, the cone C_z is polyhedral and, then, it can be characterised by a finite set of extremal rays.

That is, any element $\psi \in \mathcal{C}_z$ can be written as $\psi = \sum_{i=1}^{k_z} t_i d_i^{(z)}$, with $t_i \geq 0$ and $d_i^{(z)} \in \mathbb{R}_+^m$ for $i = 1, \dots, k_z$. Alternatively, in a more compact form, $\psi = D_z t$, $t \geq 0$, with $D_z = (d_1^{(z)} d_2^{(z)} \cdots d_{k_z}^{(z)})$.

Now, since these rays belong to the boundary of C_z , the cardinality of each of them is smaller than m. Moreover, the minimal cardinality that allows to satisfy the condition $V^T Z \psi = 0$ is n+1. Here, it is conjectured, but not proven, that there exists a set of extremal directions $d_i^{(z)}$, $i=1,\ldots,k_z$, all with cardinality n+1. In that case, the sparsity pattern of these vectors is completely determined by the signature of z.

Indeed, consider, firstly, the case m=n+1. As it has already been shown, for \mathcal{C}_z to not be degenerate it is necessary that the last elements of z is positive and that z has exactly n sign changes. In that case \mathcal{C}_z consists in exactly one dimensional ray: $\mathcal{C}_z = \{\gamma d_1^{(z)} \mid \gamma \geq 0\}$, with the elements of $d^{(z)}$ strictly positive. For the remaining cases, n+1 < m, consider a vector $\psi \in \mathcal{C}_z$ with cardinality n+1: $\psi = S_\tau \tilde{\psi}$ for some $\tau \in [m,n+1]$ and with $\tilde{\psi}$ having strictly positive elements. Then, $\tilde{\psi}$ should satisfy the constraint $V^T S_\tau \tilde{Z} \tilde{\psi} = 0$, where $\tilde{Z} = S_\tau^T Z S_\tau$ is the diagonal matrix corresponding to $\tilde{z} = S_\tau^T z$. Now, in order to have $\tilde{\psi} > 0$, it is necessary that \tilde{z} has n sign changes and ends with a non-negative element. This means that the sparsity pattern τ of the direction ψ needs to be consistent with that constraint.

Once the sparsity pattern τ is fixed, the directions can be computed as a positive solution to linear system $V^T Z S_{\tau} \psi = 0$. Choosing a positive base for that solution set provides a suitable set of extremal directions corresponding to the sparsity pattern τ .

Example 3.23. As an example, assume that the signature of z is (-+-+++), which implies that m=6 and n=3. Since all the vectors $Zd_i^{(z)}$, $i=1,\ldots,k_z$, need to have n sign changes and cardinality n+1, the matrix D_z has the sparsity structure, modulo columns permutations, given by

$$D_z = \begin{pmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & 0 & 0 \\ 0 & \times & 0 \\ 0 & 0 & \times \end{pmatrix}, \qquad z \stackrel{sign}{=} \begin{pmatrix} -\\ +\\ -\\ +\\ +\\ +\end{pmatrix}.$$

Example 3.24. If m = 9, n = 4 and $z \stackrel{sign}{=} (+ - - + + - + + +)$, then

the sparsity structure of D_z is given by

Notice that, the number of extreme directions, k_z , is given by the product of the lengths of sign-concordant sections of z. For instance, in Example 3.24 z has sections of lengths l=(1,2,2,1,3), then $k_z=\prod_{j=1}^{n+1}l_j=12$. Since z has n sign changes, l, the vector with these lengths, has n+1 elements which sums to m. Furthermore, $k_z \geq m-n$.

Consider the $m \times k_z$ matrix ZD_z . The matrix D_z can be chosen so that this matrix is only function of the signature of z and not of the values of its elements. Indeed, the columns of that matrix are extremal rays of the convex cone $\{a \in \mathbb{R}^m \mid V^T a = 0, a_i z_i \geq 0, i = 1, \dots, m\}$. Let call the resulting matrix $A(\operatorname{sign}(z))$. Note also that $A(\operatorname{sign}(z))$ is constant inside each of the cells represented in Figures 2 and 3. The cone C_z can then be written as $C_z = \{\psi = Z^{-1}A(\operatorname{sign}(z))t \mid t \geq 0\}$.

4. Discussion and examples.

4.1. Negative Shrinkages. Let assume that y has cardinality n, that is $y = S_{\tau}y_{\tau}$ for some $\tau \in [m, n]$. From (5) it follows that, whenever n is even and $\lambda_i \gg \max_{j \in \tau} \lambda_j$, the *i*-th shrinkage factor can become negative (and eventually large). The most extreme behaviour arises when τ selects the smallest eigenvalues as considered in the following result.

Lemma 4.1. Let $\tau = \{m - n + 1, ..., m - 1, m\}$, then the following bounds hold for the *i*-th element of $\omega_{(\tau)}$:

$$\omega_{(\tau),i} < 1 - (c-1)^n < 1,$$
 for $i \notin \tau$ and n even,
 $\omega_{(\tau),i} > 1 + (c-1)^n > 1,$ for $i \notin \tau$ and n odd,

with
$$c = \frac{\lambda_{m-n}}{\lambda_{m-n+1}} > 1$$
.

Corollary 4.2. If c > 2 then $\omega_i < 0$ for $i \notin \tau$.

In [19] the authors resumed their analysis reporting a table analogous to Table 4. However, they were not able to fill the bottom-left cell. Here, Lemma 4.1 allows to derive that result too. More precisely, the scaling is smaller or larger than unity depending on wether n is even or odd.

Table 4

The size of the i-th shrinkages ω_i as determined by λ_i and y_i for extreme cases.

	$ y_i \simeq 0$	$ y_i $ large
λ_i small	$\omega_i \le 1$	$\omega_i \leq 1$
λ_i large	$(-1)^n(\omega_i - 1) \le 0$	$\omega_i \simeq 1$

Note that, since ω is a smooth function of y, a similar situation arise whenever y is near to that corner point. The following numerical example, shows that large negative shrinkages can be observed also in situations not so extreme as those prescribed by the sufficient condition presented of Lemma 4.1.

Example 4.3. Consider the following setup as an exemplification of the above statements. The regression model comprises a set of m=5 explanatory variables with correlations given by $\rho_{ij}=e^{-\frac{1}{3}|i-j|}$, $i,j=1,\ldots,5$. Numerically, these correlations and the corresponding eigenvalues are given by

$$\begin{split} \rho_{1,:} &= \begin{pmatrix} 1 & 0.717 & 0.513 & 0.368 & 0.264 \end{pmatrix} \\ \lambda &= \begin{pmatrix} 3.185 & 0.981 & 0.411 & 0.241 & 0.181 \end{pmatrix}. \end{split}$$

Note setting is not at all extreme. Indeed, the condition number of the correlation matrix is 17.6 and the mean absolute correlation is just 0.54. Shrinkages for each corner point $\omega_{(\tau)}$ and for n=2,3,4 are shown in Table 5. That table reports also the value of the statistics $\widehat{\text{GDoF}}$ and $\widehat{\text{GDoF}}_{DP}$ wich will be introduced in the next section.

Here, for n = 3 and $\tau = \{1, 4, 5\}$ a consistent negative expansion ($\omega_2 = -8.41$) occurs also in a situation different from the ones suggested in the sufficient condition of Lemma 4.1.

Recall that, by Theorem 2.3 the shrinkage vector ω is a weighted average of the $\omega_{(\tau)}$ with weights being function of the observation vector y. Therefore, the large values of the shrinkages that arise at some of the points $\omega_{(\tau)}$ may have a consistent effect even when the actual ω is not to much near to these corner points.

Table 5 $\label{eq:table 5} \textit{Values for shrinkages and for the dof estimators when the y has cardinality } n.$

n	au	$\omega_{(au)}$					$\widehat{\mathrm{GDoF}}$	$\widehat{\mathrm{GDoF}}_{DP}$
2	{1,2}	1.00	1.00	0.49	0.30	0.23	3.03	3.67
	$\{1,3\}$	1.00	1.96	1.00	0.62	0.47	5.05	3.65
	$\{1,\!4\}$	1.00	3.12	1.61	1.00	0.76	7.50	0.05
	$\{1,\!5\}$	1.00	4.06	2.11	1.31	1.00	9.48	-5.70
	$\{2,3\}$	-14.15	1.00	1.00	0.69	0.54	-10.92	-224.84
	$\{2,\!4\}$	-26.40	1.00	1.41	1.00	0.80	-22.19	-745.85
	$\{2,5\}$	-36.27	1.00	1.74	1.25	1.00	-31.28	-1384.77
	$\{3,\!4\}$	-81.42	-3.27	1.00	1.00	0.86	-81.83	-6807.00
	$\{3,5\}$	-111.13	-5.15	1.00	1.14	1.00	-113.14	-12605.62
	$\{4,5\}$	-201.77	-12.60	0.10	1.00	1.00	-212.27	-41297.69
3	$\{1,2,3\}$	1.00	1.00	1.00	0.71	0.57	4.28	4.73
	$\{1,2,4\}$	1.00	1.00	1.36	1.00	0.81	5.16	4.84
	$\{1,2,5\}$	1.00	1.00	1.64	1.23	1.00	5.88	4.53
	$\{1,3,4\}$	1.00	-1.95	1.00	1.00	0.87	1.92	-3.73
	$\{1,3,5\}$	1.00	-3.26	1.00	1.13	1.00	0.87	-13.13
	$\{1,4,5\}$	1.00	-8.41	0.22	1.00	1.00	-5.19	-84.13
	$\{2,3,4\}$	185.97	1.00	1.00	1.00	0.89	189.85	-34208.14
	$\{2,3,5\}$	252.63	1.00	1.00	1.10	1.00	256.73	-63310.82
	$\{2,4,5\}$	456.04	1.00	0.48	1.00	1.00	459.52	-207058.06
	${3,4,5}$	1369.96	19.9	1.00	1.00	1.00	1392.86	-1.87×10^{6}
4	$\{1,2,3,4\}$	1.00	1.00	1.00	1.00	0.89	4.89	4.99
	$\{1,2,3,5\}$	1.00	1.00	1.00	1.10	1.00	5.10	4.99
	$\{1,2,4,5\}$	1.00	1.00	0.55	1.00	1.00	4.55	4.79
	$\{1,3,4,5\}$	1.00	14.07	1.00	1.00	1.00	18.07	-165.86
	$\{2,3,4,5\}$	-3071.07	1.00	1.00	1.00	1.00	-3067.07	-9.44×10^6

4.2. On the Degrees of Freedom of the PLS estimator. Shrinkages represent natural tools for the study of the prediction properties of the PLS estimator. Indeed, the sensitivities of the prediction vector \hat{y} with respect to changes on the actual observations are given by the Jacobian

(19)
$$J = \frac{\partial \hat{y}}{\partial y^T} = (I - 2P)\Omega + 2P.$$

As a measure of that sensitivity, the Generalised DoF (GDoF) has been introduced in [7, 26] and is given by GDoF = E[tr(J)]. The GDoF represents an extension of DoF concept to non linear estimators. The use of that measure for PLS regressions was advocated in [17] where the authors propose its sample counterpart as an unbiased estimator for GDoF. The need for an estimator for the DoF arise, for instance, in the estimation of the disturbance or prediction error variances or for determining the number of directions to

be used by PLS. The alternative measure $GDoF_{DP} = E[tr(2J - J^T J)]$, for the DoF of PLS have been proposed in [5, 23], while other measures based on cross validation have also been considered (see for instance [25]).

Consider now, the behaviour of this DoF estimator in the situations identified in the previous subsection. Assume that y has cardinality n, that is $y = S_{\tau}y_{\tau}$ for an appropriate τ . Under this setup, the projection P can be rewritten as $P = S_{\tau}S_{\tau}^{T}$ and the estimators for the degree of freedom become

$$\widehat{\text{GDoF}} = \operatorname{tr}\left(\Omega + 2S_{\tau}S_{\tau}^{T}(I - \Omega)\right) = n + \sum_{i \notin \tau} \omega_{i},$$

and

$$\widehat{GDoF}_{DP} = \operatorname{tr}\left(I - (I - \Omega)^2\right) = m - \sum_{i \notin \tau} (1 - \omega_i)^2.$$

Then, if n is even and the assumptions of Lemma 4.1 are satisfied with c>2, then $\widehat{\mathrm{GDoF}}< n$. Clearly, alternative values of c could also lead to a negative $\widehat{\mathrm{GDoF}}$ or to a value exceeding the number of observations. Moreover, if the density of y is concentrated enough around $S_{\tau}\mu_{\tau}$, the same conclusions can be drawn for the actual GDoF. Analogously, meaningless values $\widehat{\mathrm{GDoF}}_{DP}$ arise in proximity of "degenerate" models where shrinkages can become very large in absolute value (see Table 5 below).

Lemma 4.1 provides a sufficient condition that contradicts a conjecture considered in [17] and "voiced" in [10, 20] which states that GDoF > n. This property, was analytically proven to hold for the first PLS step and empirically confirmed by means numerical experiments for the remaining ones [17]. It is also worth noting that, negative values for $\widehat{\text{GDoF}}$ were indeed observed in the experiment of Kramer and Sugiyama for large model dimensions (see [17] Section 4.3). Nonetheless, this behaviour was attributed to numerical instabilities that characterises Krylov methods and which are likely to occur for high-dimensional models. Even if the numerical instability of this class of methods is here recognised, we believe that most the these negative DoFs are the effects a mechanism similar to the one here discussed. Indeed, as m increases it is more likely to have y orthogonal to a consistent set of principal axes, that is, to observe a shrinkage vector located near a corner of the domain region.

A clear example of this behaviour can be seen in Example 4.3. In that setup, computing the estimator for the DoF when y = (1, 0, 0, 1, 1) at the 3-rd iteration of the PLS gives an estimate $\widehat{\text{GDoF}} = -5.18843$ (see Table 5).

Looking at Table 5, it is clear that things can go much worse, this DoF measure can become extremely large and either positive or a negative.

Example 4.4 (continuation of Example 4.3). The cases reported in Table 5 are cases of exact under-specification. Indeed, when the cardinality of y is equal to n, the PLS method has found the OLS estimator and thus there may be no reason to look at the sensitivity w.r.t. null elements of y. To analyse a less extreme situation, using the same model matrix, consider a setup where $y = \Lambda \beta$, with

$$\beta = \begin{pmatrix} 0.10 & 0.01 & 0.01 & 5.00 & 5.00 \end{pmatrix}.$$

For that observation vector the estimates of the DoF for the 3rd step of PLS (n=3) is given by $\widehat{\mathrm{GDoF}} = -3.134$.

Now, in order to consider a proper inferential setup, the above example is extended to the regression $y = \Lambda \beta + \varepsilon$, where the additional disturbance vector is normally distributed: $\varepsilon \sim N(0, \sigma^2 \Lambda)$, with $\sigma = 0.02$. Being unable to derive an explicit expression for the distribution of $\widehat{\mathrm{GDoF}}$, a Monte Carlo (MC) experiment with 20000 replications from the model has been performed. The resulting value for $\widehat{\mathrm{GDoF}} = \widehat{\mathrm{E}}[\widehat{\mathrm{dof}}]$ is -0.461 with an MC error having standard deviation of 0.026. The result is less sharp than in the previous estimate, but still it is negative and consequently smaller than n. The empirical distribution function of $\widehat{\mathrm{GDoF}}$ is reported in Figure 4 and MC estimation for the probability $\widehat{\mathrm{P}}[\widehat{\mathrm{GDoF}} < 0]$ is 0.56. Figure 4 reports also the empirical distribution of $\widehat{\mathrm{GDoF}}_{DP}$ showing the pour performances of that estimator.

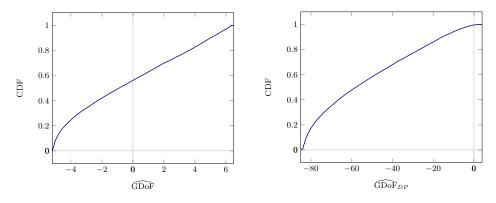


FIG 4. CDF of the GDoF and GDoF_{DP} when $\lambda = (3.18, 0.98, 0.41, 0.24, 0.18), \beta = (0.1, 0.01, 0.01, 5, 5), \sigma = .02$ and n = 3 and estimated by a MC experiment with 20 000 replications.

5. Conclusions. A precise characterisation of the geometrical structure of PLS shrinkages is here provided. The proposed analysis encompass and complete a part of the literature on PLS regression [1, 10, 11, 14, 19, 16]. Here, the shrinkage vector is expressed as a weighted average of a set of basic vectors that do not depend on the observations. That expression is a generalisation of the one considered in [1] for a couple of special cases. Also, this analysis allowed to complete the one proposed in [19] where one extreme situation could not be addressed. The explicit expression here proposed may represent a starting point for the derivation of the distributions needed for performing inference with PLS regression estimators. To this end, the author remarks that the domain of the shrinkage vector variable has been here formally and completely characterised. Moreover, the inverse image of the shrinkage function is provided. This result provides a starting step for the derivation of the distribution of the shrinkage factors.

Furthermore, regions where the PLS regression estimator has an highly non-linear behaviour and very large shrinkages (in absolute value) have been characterised. In these situations, recently proposed measures of the DoF for non-linear estimators completely fail as they provide unrealistic results such as extremely large or negative values. The analytic tools here derived allowed to prove that the conjecture stating that the PLS estimator always uses more "DoF" than the number of PLS directions does not generally hold [10, 17, 20]. To this end, a sufficient condition and some counterexamples have been provided. The failure of the "GDoF" statistic [7, 17, 26] here identified points to the need of a deeper reflection on the DoF concept especially in highly non-linear contexts.

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