Group-sparse block PCA and explained variance

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Abstract

The paper addresses the simultaneous determination of group-sparse loadings by block optimization, and the correlated problem of defining explained variance for a set of non orthogonal components. We give in both cases a comprehensive mathematical presentation of the problem, which leads to propose i) a new formulation/algorithm for group-sparse block PCA and ii) a framework for the definition of explained variance with the analysis of five definitions. The numerical results i) confirm the superiority of block optimization over deflation for the determination of group-sparse loadings, and the importance of group information when available, and ii) show that ranking of algorithms according to explained variance is essentially independant of the definition of explained variance. These results lead to propose a new optimal variance as the definition of choice for explained variance.

Keywords: Sparse PCA, group variables, block optimisation, explained variance.

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Introduction

Most of the algorithms developed in the recent years for sparse PCA aim at determining one single sparse principal component, and rely on the deflation process inherited from the unconstrained PCA when it comes to compute more than one sparse principal component [5], [10], [13], [17], [14], [11].

However, the use of the PCA deflation scheme in the sparse context where loadings and components are not necessarily orthogonal can lead to difficulties [8]. Some authors, also motivated by the fact that joint optimization with respect to all loadings is expected to be more effective for variance maximization than sequential optimization, have tried to determine all loadings simultaneously: Zou et al. [18] solve sparse PCA as a regression type problem, and Journé et al. [7] use a block dual approach to sparse PCA.

Our contribution in this paper is twofold. We give first a new comprehensive presentation of the block $\ell_1$-algorithm of [7], which we generalize at the same time to the case where sparsity is required to hold on group of variables (group variables) rather than on the individual variables (scalar variables); this leads to a new group-sparse block PCA algorithm, for which we propose a strategy for the choice of the sparsity inducing parameters. We compare numerically the performance of block and deflation algorithms for group-sparse PCA on synthetic data with four sparse underlying loading vectors. Then we illustrate the influence of the group information on the retrieval of the sparsity pattern.

The second aspects concerns the quality assessment of a sparse principal component analysis in term of explained variance. Two definitions have been proposed in the literature for explained variance: the adjusted variance of Zou [18] and the total variance of Shen et al. [14], but there was no systematic study on the subject. So we define in this paper a framework for the definition of explained variance for a set of non necessarily orthogonal components, which leads us to introduce three additional definitions. We investigate the mathematical properties of these five “natural” definitions, in particular their relative magnitudes, and check whether they are guaranteed to be smaller than the explained variance for non sparse PCA (sum of squared singular values). Numerical experimentation confirms the theoretical results, and show that the ranking of algorithms is essentially independant of the chosen definition of explained variance.

The proposed Group-Sparse Block algorithms and the explained variance functions are implemented in a R package “sparse PCA” and are available
at the URL https://github.com/chavent/sparsePCA.

The paper is organized as follows: we recall in section 1 the equivalent deflation and block formulations of non sparse PCA. In section 2 we generalize the above block formulations to the search of group-sparse loadings, which leads to the introduction and analysis of the proposed group-sparse block PCA algorithm. The performances of the block and group-sparse features of the new algorithm are evaluated numerically against deflation in section 3. Section 4 is a mathematical section devoted to the problem of defining explained variance for a set of non necessarily northogonal components. Magnitude and ranking properties of the various definitions are studied numerically in section 5.

1 Principal Component Analysis

We recall in this section the deflation and three block formulation of PCA for the case of \(|p|\) scalar variables (we save the notation \(p\) for the number of group variables from section 2 on).

Let \(A\) be the data matrix of rank \(r\), whose \(n \times |p|\) entries are made of \(n\) samples of \(|p|\) centered variables, and \(\|\cdot\|_F\) denote the Frobenius norm on the space of \(n \times |p|\) matrices:

\[
\|A\|_F^2 = \sum_{i=1}^{n} \sum_{j=1}^{|p|} a_{ij}^2 = \text{tr}(A^T A) = \sum_{j=1}^{r} \sigma_j^2 ,
\]

where the \(\sigma_j\)'s are the singular values of \(A\), defined by its singular value decomposition:

\[
A = U \Sigma V^T \quad \text{with} \quad U^T U = I_r , \quad V^T V = I_r , \quad \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_r) = r \times r \text{ matrix with } \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0 .
\]

The columns \(u_1 \ldots u_r\) of \(U\) and \(v_1 \ldots v_r\) of \(V\) are the left and right singular vectors of \(A\).

Principal Component analysis (PCA) searches for a number \(m \leq r\) of combinations \(z_j, j = 1, \ldots, m\) (loading vectors) of the \(|p|\) variables such that the variables \(y_j = Az_j, j = 1 \ldots m\) (components) are uncorrelated and explain an as large as possible fraction of the variance \(\|A\|_F^2\) of the data. The optimal loadings and component are given by:

\[
z_j^* = v_j , \quad j = 1 \ldots m \quad (m \text{ first right singular vectors of } A) ,
\]

\[
y_j^* = Av_j = \sigma_j u_j \quad (\text{proportional to } m \text{ first left singular vectors of } A) ,
\]
and the part of the variance explained by these components is:

\[
\text{var}\{y^*_1, \ldots, y^*_m\} = \sum_{j=1}^{m} \|y_j\|^2 = \sum_{j=1}^{m} \sigma^2_j \leq \sum_{j=1}^{r} \sigma^2_j = \|A\|_F^2.
\]

1.1 The deflation approach

One is usually interested in the few components associated to the largest singular values of \(A\). Hence a widely used solution to PCA is Hotelling’s deflation \[^{12}\], where the singular vectors are computed successively by recurrence:

\[
\begin{align*}
A_0 & = A, \ z_0 = 0, \ 	ext{and compute, for } j = 1 \ldots m: \\
A_j & = A_{j-1}(I_{|p|} - z_{j-1}z_{j-1}^T) \\
z_j & = \underset{\|z\|=1}{\text{argmax}} \|A_jz\|^2
\end{align*}
\]

The \(m\) first singular values and singular vectors are then given by:

\[
\begin{cases}
\quad v_j = z_j, \ j = 1 \ldots m, \\
\quad \sigma_ju_j = Av_j \quad \text{with} \quad \|u_j\| = 1, \ \sigma_j \geq 0, \ j = 1 \ldots m.
\end{cases}
\]

In this approach, the errors accumulate along the computations, and the precision on \(v_j\) and \(\sigma_j\) is expected to get worse when \(j\) increases, which is not a problem when only a small number of components is computed.

1.2 Block PCA formulations

In opposition, block PCA formulations search simultaneously for the \(m\) loadings \(z_j\) and/or the \(m\) normalized components \(x_j\). We define to this effect three block unknowns:

\[
\begin{align*}
Z & = [z_1 \ldots z_m] \in \mathbb{R}^{|p| \times m} \text{ (tentative loadings)}, \\
Y & = [y_1 \ldots y_m] \in \mathbb{R}^{n \times m} \text{ (tentative components)}, \\
X & = [x_1 \ldots x_m] \in \mathbb{R}^{n \times m} \text{ (tentative normalized components)}.
\end{align*}
\]

With these notations, the solution \[^{3} \quad ^{4}\] to the PCA problem is:

\[
\begin{align*}
Z^* = [v_1, \ldots, v_m], \ Y^* = [\sigma_1u_1, \ldots, \sigma_mu_m], \ X^* = [u_1, \ldots, u_m].
\end{align*}
\]
One defines then three block objective functions:

\begin{align*}
  f_L(Z) &= \sum_{j=1}^{m} \mu_j^2 \|Az_j\|^2 = \text{tr}\{Z^T A^T AZ N^2\}, \\
  f_C(X) &= \sum_{j=1}^{m} \mu_j^2 \|A^T x_j\|^2 = \text{tr}\{X^T A A^T X N^2\}, \\
  f_{CL}(X, Z) &= \sum_{j=1}^{m} \mu_j^2 (x_j^T Az_j)^2,
\end{align*}

where the subscripts L and C remind of the nature of the arguments of the function (L for loadings Z or/and C for the (normalized) components X), and where N is a diagonal matrix of weights \(\mu_j\) chosen such that:

\begin{equation}
  N = \text{diag}\{\mu_1, \ldots, \mu_m\} \quad \text{with} \quad \mu_1 > \mu_2 > \cdots > \mu_m > 0.
\end{equation}

Depending on the formulation, we shall require that the \(|p| \times m\) unknowns Z and the \(n \times m\) unknowns X retain some properties of the right and left singular vectors. So we define, for \(k = |p|\) or \(n\), the set of \(k \times m\) matrices with columns in the unit ball:

\begin{equation}
  (B^k)^m = \{N \in \mathbb{R}^{k \times m} \text{ such that } \|n_j\|^2 \leq 1, \ j = 1 \ldots m\}
\end{equation}

and the set of \(k \times m\) matrices with orthonormal columns (Stiefel manifold):

\begin{equation}
  S_k^{m} = \{O \in \mathbb{R}^{k \times m} \text{ such that } O^T O = I_m\}.
\end{equation}

This leads to define four constrained optimization problems with respect to the block unknowns Z and/or X:

\begin{align*}
  (18) & \quad \max_{Z \in S_m^p} f_L(Z) \quad \text{(loading formulation)}, \\
  (19) & \quad \max_{Z \in S_m^p, X \in (B^n)^m} f_{CL}(X, Z) \quad \text{(loading/component formulation)}, \\
  (20) & \quad \max_{X \in S_m^n} f_C(X) \quad \text{(component formulation)}, \\
  (21) & \quad \max_{X \in S_m^n, Z \in (B^p)^m} f_{CL}(X, Z) \quad \text{(component/loading formulation)},
\end{align*}

where the orthonormality constraint is imposed on Z in the two first formulations, and on X in the two last.
Proposition 1.1 Let the singular values of $A$ satisfy:

\begin{equation}
\sigma_1 > \sigma_2 > \cdots > \sigma_m > 0,
\end{equation}

and the weights $\mu_j$ satisfy (15). Then the solution $Z^*$ and $X^*$ of the PCA problem given by (11) is the unique solution (up to a multiplication by $\pm 1$ of each column of course) of the optimization problems (18), (19), (20) and (21), Moreover:

\begin{equation}
f_L(Z^*) = f_{CL}(X^*, Z^*) = f_C(X^*) = \sum_{j=1}^{m} \mu_j^2 \sigma_j^2,
\end{equation}

Because they are the singular vectors of $A$, the maximizers $Z^*$ and $X^*$ are independant of the weight $\mu_j$, so that:

\begin{equation}
\text{the variance explained by } Y^* = AZ^* \text{ is } \text{var}Y^* = \sum_{j=1}^{m} \sigma_j^2,
\end{equation}

and:

\begin{equation}
x_j^* = (Az_j^*)/\|Az_j^*\|, \quad z_j^* = (A^Tx_j^*)/\|A^Tx_j^*\| \quad \text{for } j = 1 \ldots m.
\end{equation}

**Proof:** The equivalence of (18) with the PCA problem and the uniqueness of the maximizer $Z^*$ is a classical result, see for example [2, 3], and Theorem 7.1 in the Appendix. The equivalence between (18) and (19) follows immediately from:

\begin{equation}
\forall z \in \mathbb{R}^{|p|}, \quad \|Az\|^2 = \max_{x \in \mathcal{B}^n} (x^TAz)^2.
\end{equation}

The rest of the proposition follows by replacing $A$ by $A^T$. 

**Remark 1.2** When $\mu_1 = \cdots = \mu_m = 1$, any $Z \in S_m^p$ which maximizes $f_L(Z)$ is a basis of the eigenspace $\text{vect}\{v_1 \ldots v_m\}$ of $A$, this is why it is necessary to use different weights to select the eigenvector basis itself. Then (15) ensures that the computed singular vectors are numbered in order of decreasing singular values when the global maximum is achieved. But depending on the initial value of $Z$ and/or $X$, local optimization algorithms may converge to a local maximum, producing thus singular vectors in a different order.
2 Group-sparse block PCA formulations

The block formulations of section 1.2 are not specially interesting for the resolution of standard PCA problems, as efficient deflation methods exist already. But we use them in this section as starting point for the construction of block formulations for group-sparse PCA. This leads to the new group-sparse block formulations which generalize to the case of group variables the sparse $\ell^1$-formulation of formule (16) page 524.

We introduce first group variables notations. From now on, we shall denote by $p$ both the number of group variables and the multi-index:

$$p = (p_1, \ldots, p_p) \quad \text{with} \quad |p| = p_1 + \cdots + p_p,$$

which describes the number of scalar variables in each group variable. There will be no ambiguity from the context. With this notation, the data matrix $A$ is an $n \times |p|$ matrix of the form:

$$A = \begin{bmatrix} a_1 & \cdots & a_p \end{bmatrix},$$

where the $a_i$'s are $n \times p_i$ matrices, and loading vectors $z_j \in \mathbb{R}^{p_i}, j = 1 \ldots m$ are of the form:

$$z_j^t = \begin{bmatrix} z_{1,j}^t \ldots z_{p,j}^t \end{bmatrix},$$

where the $z_{i,j}$'s are column vectors of dimension $p_i$. We denote by $\| \|_2$ the norm on $n \times p_i$ matrices induced by the Euclidian norms $\| \|$ on $\mathbb{R}^n$ and $\mathbb{R}^{p_i}$ (largest singular value):

$$\|a_i z_{i,j}\| \leq \|a_i\|_2 \|z_{i,j}\| \quad \forall z_{i,j} \in \mathbb{R}^{p_i}.$$

2.1 Three group-sparse formulations

In order to promote the apparition of zeroes in the loading vectors for some group variables, we define the group $\ell^1$-norm of the loadings $z_j$ by:

$$\|z_j\|_1 = \sum_{i=1}^p \|z_{i,j}\|, \quad j = 1 \ldots m,$$

where $\|z_{i,j}\|$ is the Euclidean norm on $\mathbb{R}^{p_i}$, and choose regularization parameters:

$$\gamma_j > 0, \quad j = 1 \ldots m.$$
We modify the block objective functions of section 1.2 in such a way that loadings matrices $Z$ with columns $z_j$ with large group $\ell_1$-norm are penalized. Among these functions, only $f_L$ defined by (12), and $f_{CL}$ defined by (14), depend on $Z$, so we define group-sparse versions of these functions by:

\[(33) \quad f^gs_L(Z) = \sum_{j=1}^{m} \mu_j^2 \left[ \|A z_j\| - \gamma_j \|z_j\|_1 \right]_+^2,\]

\[(34) \quad f^gs_{CL}(X, Z) = \sum_{j=1}^{m} \mu_j^2 \left[ x_j^T A z_j - \gamma_j \|z_j\|_1 \right]_+^2,\]

where $[t]_+ = t$ if $t \geq 0$ and $[t]_+ = 0$ if $t < 0$. The block PCA formulations (18), (19), (21) lead then to three group-sparse block PCA formulations:

\[(35) \quad \max_{Z \in S_m^{[p]}} f^gs_L(Z) \quad \text{(group-sparse loading formulation)},\]

\[(36) \quad \max_{Z \in S_m^{[p]}} \max_{X \in (B^n)^m} f^gs_{CL}(X, Z) \quad \text{(group-sparse loading/component formulation)},\]

\[(37) \quad \max_{X \in S_m^{[n]}} \max_{Z \in (B^p)^m} f^gs_{CL}(X, Z) \quad \text{(group-sparse component/loading formulation)},\]

We discuss first the mathematically equivalent formulations (35) and (36). By construction, $f^gs_L$ and $f^gs_{CL}$ have the same maximizing loading vectors $z_j^*$, and the maximizer $X^* = [x_1^* \ldots x_m^*]$ in (36) satisfies (compare to (25)):

\[(38) \quad x_j^* = (A z_j^*)/\|A z_j^*\|, \quad j = 1 \ldots m.\]

This shows that the vectors $x_j^*$ are the normalized components associated to $z_j^*$. Hence the two formulations (35)(36) produce orthonormal sparse loading vectors $z_j^*$’s, and the associated normalized components $x_j^*$’s - which, of course, are not necessarily orthogonal when the sparsity parameter $\gamma$ is active (at least one $\gamma_j > 0$). Hence these formulations are appealing from the point of view of sparse PCA, as they reconcile sparsity with orthonormality of at least the loading vectors. However, they combine the difficulties associated to the orthonormality constraint on $[z_1^* \ldots z_m^*]$ with the presence of the non-differentiable group $\ell_1$-norm terms $\|z_j\|_1$ in the objective function. Optimization algorithms exist which take care of each difficulty separately, see
for example, for the orthonormality constraint, [2], and [7, Algorithm 1 page 526] recalled in section 7.2 of the Appendix, and, for the $\ell^1$-regularization, subgradient methods [13]. But solving both difficulties simultaneously is a delicate problem, which is left to further studies.

In opposition, the third formulation (37) is not anymore equivalent to (35)-(36) as soon as $m > 1$. It produces non necessarily orthonormal sparse loading vectors $z_j^*$’s, and orthonormal vectors $x_j^*$’s - but these latter do not coincide anymore with the normalized component:

\[ x_j^* \neq (Az_j^*)/\|Az_j^*\|, \quad j = 1 \ldots m, \]

in opposition to (25) in the case where no sparsity is required.

Hence neither the sparse loading vectors nor the principal components produced by formulation (37) are orthogonal, which is less satisfying from the point of view of PCA. But the good side of this formulation is that the numerical difficulties are split between $X$ and $Z$ : the orthonormality constraint is for $X$, the non-differentiable group $\ell^1$-norm is for $Z$ ! Moreover, as it was shown, for scalar variables, first by d’Aspremont et al. [4] in the case of cardinality regularization, and by Journé in [7] in the case of $\ell^1$ regularization, the inner maximization loop on $Z$ in (37) can be solved analytically for any given $X \in S_{nm}^n$, despite the non-differentiable terms, thus leading to the maximization of the differentiable convex function of $X$:

\[ X \rightsquigarrow F(X) \overset{\text{def}}{=} \sum_{j=1}^m \mu_j^2 \bar{\sum}_{i=1}^p \left[ \|a_i^T x_j\| - \gamma_j \right]_+^2. \]

For scalar variables ($p_j = 1, j = 1 \ldots p$), $F(X)$ coincides with the function $\Phi^2_{\ell_1,m}$ of Journé et al. [7, formula (16) page 524]. Hence formulation (37) generalizes to group variables the block sparse PCA via $\ell_1$–Penalty method of [7], and we restrict ourselves in the sequel to formulation (37).

### 2.2 Resolution of the group-sparse component/loading block formulation (37)

We recall the polar decomposition of a $k \times \ell$ matrix $G$:

\[ G = UP, \]

where $U$ is a $k \times \ell$ unitary matrix ($U^T U = I_\ell$) - not to be confused with the matrix $U$ in the SVD of $A$, and $P$ is a positive $\ell \times \ell$ semidefinite matrix.
\( P \geq 0 \). The matrix \( U \) is called the polar matrix of \( G \) :

\[
(42) \quad U = \text{polar}(G).
\]

When \( G \) happens to be a vector, \( U \) is simply the unit vector pointing in the direction of \( G \) (or any unit vector if \( G = 0 \)), and \( P \) is the norm of \( G \).

For any \( X = [x_1 \ldots x_m] \in S^n_m \) and any \( i = 1 \ldots p, j = 1 \ldots m \) we introduce the polar decomposition (cf (41)) of \( a^T_i x_j \in IR^p \):

\[
(43) \quad a^T_i x_j = u_{ij} \alpha_{ij}, \text{ with } \|u_{ij}\| = 1, \quad \alpha_{ij} \geq 0,
\]

and define for \( j = 1 \ldots m \) the vectors \( t_j = (t_{ij}, i = 1 \ldots p) \) of \( IR^p \) by :

\[
(44) \begin{cases}
    t_{ij} = u_{ij}(\alpha_{ij} - \gamma_j)_+ \in IR^p, & i = 1 \ldots p, \\
    \|t_j\|^2 = \sum_{i=1}^p (\alpha_{ij} - \gamma_j)_+^2.
\end{cases}
\]

When \( \gamma_j \to 0 \), one sees that \( t_j \to A^T x_j \), so \( t_j \) can be understood as a perturbation of \( A^T x_j \) caused by the sparsity inducing parameter \( \gamma_j \).

**Proposition 2.1** The solution \((X^* Z^*)\) of (37) can be obtained in two steps :

1. determine \( X^* = [x_1^* \ldots x_m^*] \) which maximizes over \( S^n_m \) the function :

\[
(45) \quad F(X) = \sum_{j=1 \ldots m} \mu_j^2 \sum_{i=1}^p (\|a_{ij}^T x_j\| - \gamma_j)_+^2 = \sum_{j=1 \ldots m} \mu_j^2 \|t_j\|^2.
\]

2. Define \( Z^* = [z_1^* \ldots z_m^*] \) by :

\[
(46) \quad \forall j = 1 \ldots m, \quad z_j^* = \begin{cases} 0 & \text{if } t_j^* = 0, \\
    t_j^*/\|t_j^*\| & \text{if } t_j^* \neq 0.
\end{cases}
\]

3. The condition :

\[
(47) \quad \min_{j=1 \ldots m} \gamma_j < \max_{i=1 \ldots p} \|a_i\|_2,
\]

ensures that at least one of the \( t_j^* \) and \( z_j^* \) are non zero, and hence that the value of the maximum in (45) is strictly positive.
The proof of this proposition is given in section 7.3 of the Appendix.

Step 1 of proposition 2.1 can be solved applying Algorithm 1 of section 7.2 of the Appendix (Journé et al. [7, page 526]) to the maximization of $F(X)$ on the Stiefel manifold $M = S^n_m$. The gradients of $F$ are given by:

\[(48) \nabla_{x_j} F(X) = 2\mu_j^2 A t_j, \quad j = 1 \ldots m,\]

or in matrix form:

\[(49) \nabla_X F(X) = 2ATN^2 \in \mathbb{R}^{n \times m} \quad \text{with} \quad T = [t_1 \ldots t_m] \in \mathbb{R}^{p \times m}.\]

The maximizer of the inner loop of Algorithm 1 is the polar of $\nabla_X F(X)$, so Algorithm 1 boils down to:

**Algorithm 2**

| input       | $X_0 \in S^n_m$ |
| output      | $X_n$ (approximate solution) |
| begin       | |
| 0 $\leftarrow k$ |
| repeat      | |
| $T_k$ $\leftarrow$ [44] |
| $G_k$ $\leftarrow$ $\nabla_X F(X_k) = 2AT_kN^2$ |
| $X_{k+1}$ $\leftarrow$ polar($G_k$) |
| $k$ $\leftarrow$ $k + 1$ |
| until a stopping criterion is satisfied |
| end         | |

### 2.3 A group-sparse deflation algorithm

In section 3 the block algorithm of previous section will be evaluated numerically against a group-sparse deflation algorithm, which we recall here for sake of completeness (compare with section 1.1):

\[(50) \quad A_0 = A, \quad z_0 = 0, \quad \text{and compute, for } j = 1 \ldots m:\]

\[(51) \quad A_j = A_{j-1}(I_{|p|} - z_{j-1}z_{j-1}^T)\]

\[(52) \quad z_j = \operatorname{argmax}_{\|z\|=1} (\|A_jz\| - \gamma_j\|z\|_1)\]

The optimization problem (52) coincides with the group-sparse block formulations (35) (36) written for $m = 1$, which in this case case coincide also with
the group-sparse component/loading formulation \cite{37}. Hence \cite{52} can be solved by the block Algorithm 2 of previous section applied to the determination of a single loading.

3 Group-sparse block Algorithm 2 : numerical results

The ability of Algorithm 2 to retrieve group-sparse singular vectors has been tested on synthetic data generated using a set of 20 unit norm right singular vectors associated to the eigenvalues values 200, 180, 150, 130, 1...1. There are hence \(|p| = 20\) scalar variables, and \(p = 5\) group variables made of \(p_j = 4, j = 1...p\) scalar variables each. The four vectors associated to the largest singular values - the “underlying loadings \(Z_{true}\)” - are group-sparse as shown in figure 1.

Using these data, we have simulated two sets of 100 data matrices \(A\), one with \(n = 300\) samples (lines), and a second with \(n = 3000\). More precisely, we have followed the procedure proposed by Shen and Huang \cite{14} and Journée et al \cite{7} to generate data matrices \(A\) by drawing \(n\) samples from a zero-mean distribution with covariance matrix \(C\) defined by \(C = V_{true} \Sigma_{true}^2 V_{true}^T\), where \(\Sigma_{true} = \text{diag}(200, 180, 150, 130, 1, \ldots, 1)\), and \(V_{true}\) is the \(|p| \times |p|\) orthogonal matrix defined by the QR-decomposition \([Z_{true}, U] = V_{true} R\), where \(U\) of dimension \(|p| \times (|p| - m)\) is randomly drawn from \(U(0, 1)\). Notice that, by definition of the QR-decomposition, the \(m\) first columns of \(V_{true}\) coincide with \(Z_{true}\).

In order to limit the odds that the algorithm converges to a local maximum and produces loadings in the wrong order, we have chosen in all numerical experiments - deflation as well as block algorithms - to use the left singular vectors \([u_1 \ldots u_m]\) as initial value \(X_0\) in Algorithm 2.
We discuss now the choice of regularization parameters: each sparsity parameter $\gamma_j$ needs to be fitted to the norm of the vector $A^T x_j$ it is in charge of thresholding. This norm is simply estimated by its initial value $\|A^T x_j\| = \|A^T u_j\| = \|\sigma_j v_j\| = \sigma_j$. To this effect we define nominal sparsity parameters $\gamma_{j,\text{max}}$ for each component by:

$$
\gamma_{j,\text{max}} = \frac{\sigma_j}{\sigma_1} \gamma_{\text{max}} \quad \text{where} \quad \gamma_{\text{max}} \overset{\text{def}}{=} \max_{i=1 \ldots p} \|a_i\|_2 \quad \text{as defined in (47)},
$$

and reduced sparsity parameters $\lambda_j$ by:

$$
\lambda_j = \frac{\gamma_j}{\gamma_{j,\text{max}}} , \quad j = 1 \ldots m .
$$

In order to place ourselves in the situation where no a priori information on the sparsity of the underlying loadings is known, we have used the same reduced parameters $\lambda$ for all loadings:

$$
\lambda = \lambda_1 = \cdots = \lambda_m ,
$$

and have explored the influence of $\lambda$ by letting it vary from 0 to 1 by steps of 0.01.

According to Remark 1.2 we have chosen strictly decreasing weights $\mu_j$, for example:

$$
\mu_j = 1/j , \quad j = 1 \ldots m ,
$$

in order to relieve the underdetermination which happens for equal $\mu_j$ at $\lambda = 0$ and to drive the optimization, when $\lambda > 0$, towards a minimizer $X^*$ which is “close” to the $m$ first left eigenvectors $[u_1, \ldots, u_m]$. Nevertheless, we have also tested the behavior of the algorithm for equal weights:

$$
\mu_j = 1 , \quad j = 1 \ldots m .
$$

We review now the different indicators at our disposal for the evaluation of the algorithms.

The adequation of the sparsity structure of the estimated loadings $Z$ to that of the underlying $Z_{\text{true}}$ is measured by:

- the true positive rate (tpr): proportion of zero entries of $Z_{\text{true}}$ retrieved as 0 in $Z$, 

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the false positive rate (fpr) : proportion of non zero entries of $Z_{true}$ retrieved as 0 in $Z$.

These quantities can be evaluated loading by loading (i.e. on the columns of $Z$), or globally over all loadings (i.e. on the whole matrix $Z$).

The subspace distance between $Z_{true}$ and $Z$ will be measured by $R_V(Z, Z_{true})$ where $R_V(X, Y)$ is the $R_V$-factor defined by [6][1] :

$$R_V(X, Y) = \frac{\|X^T Y\|_F^2}{\|X^T X\|_F \|Y^T Y\|_F} = \frac{\langle X^T X, Y^T Y \rangle_F}{\|X^T X\|_F \|Y^T Y\|_F} = R_V(Y, X).$$

The first formula is used to compute $R_V$, and the second implies that :

$$0 \leq R_V(X, Y) \leq 1.$$  \hfill (58)

The orthogonality of components will be measured by the $m$-dimensional volume of the parallelepiped constructed on the columns of $Y$, which is the absolute value of the determinant of the $m \times m$ matrix whose entries are the coordinates of $y_1 \ldots y_m$ on any orthonormal basis of the subspace they span. For example, if one performs a QR decomposition of $Y$, this volume is given by $|\text{det}(R)| = \prod_{j=1}^{m} r_{j,j}$. In order to obtain a dimensionless measure of orthogonality, we divise this volume by that of the rectangular parallelepiped with edges of length $\|y_j\|$, which leads us to measure the orthogonality of $Y$ by :

$$0 \leq \text{vol}(Y) = \frac{\prod_{j=1}^{m} r_{j,j}}{\prod_{j=1}^{r} \|y_j\|} \leq 1.$$  \hfill (60)

3.1 Block versus deflation

We compare here the performance of three group-sparse algorithms :

- deflation : the deflation algorithm described in section 2.3
- block_different_mu : the block Algorithm 2 of section 2.2 with $\mu_j = 1/j$
- block_same_mu : as above but with $\mu_j = 1$ for all $j$.

We have represented in figure 2 the mean values of tpr and fpr for the loadings resulting from the application of the three algorithms to the 100 $A$ matrices
computed from 300 samples (left) and 3000 samples (right). The sparsity pattern is perfectly recovered for the values of $\lambda$ such that $\text{tpr} = 1$ and $\text{fpr} = 0$!

When 3000 samples are available, both the deflation algorithm and the block algorithm with different $\mu$ are able to retrieve, even in the mean, the exact sparsity structure of $Z_{\text{true}}$ for $\lambda \approx 0, 1$, whereas the block algorithm with same $\mu$ tends to add too many zeros at wrong places even for small values of $\lambda$.

When only 300 samples are available, the problem is more difficult, and the block algorithm with different $\mu$ takes advantage on the deflation algorithm, whose $\text{tpr}$ grow slower and $\text{fpr}$ grow faster with $\lambda$. And, as in the previous case, the the block algorithm with same $\mu$ performs the worst with its tendency to add too quickly wrong zeroes.
1.1 Graphiques de vérité par dimension
1.1.1 tpr et fpr en fonction de lambda

deflation, n=300

block, different μ, n=300

block, same μ, n=3000

Figure 2: Mean true positive rates (dotted lines) and false positive rates (full lines) for each sparse loading versus reduced sparsity parameter $\lambda$. From top to bottom: deflation, block, different μ, block, same μ. Left: 300 samples, right: 3000 samples.
The boxplots of figure 3 show the median and the variability of the global tpr and fpr with the realisations of the data matrix $A$, for $\lambda = 0, 1$ (top) and $\lambda = 0, 2$ (bottom). As expected, increasing $\lambda$ increases the global true positives, at the expense of more false positive. In the two cases, the deflation and block_different_mu algorithms exhibit similar false positive rates medians, but the latter shows a higher true positive rate median of less dispersion. The block_same_mu algorithm does not seem practically usable, as it finds false positives even for quite small values of $\lambda$.

Figure 3: Variability of global true positive rates (left) and false positive rates (right) for each algorithm: deflation, block_different_mu, block_same_mu, in the case of 300 samples; top: $\lambda = 0, 1$, bottom: $\lambda = 0, 2$.

The orthogonality level of components $Y$ and the RV-distance of loadings $Z$ to the underlying $Z_{true}$ are shown in figure 4. Here again, the block_different_mu algorithm performs better than deflation, at the prize of a barely worse orthogonality default of the components.
Finally we check the performance of the three algorithms against the levels of optimal and adjusted variance explained by the sparse components (see section 4, formulas (94) and (93). We display in Figure 5 the corresponding proportion of explained variance pev defined by (107). One sees that block algorithms produce a higher proportion of explained variance than the deflation algorithm. However, this has to be tempered by the fact that differences in pev are less than 0,01, within the ranking uncertainty of the explained variance definitions (see section 5.2 below). Nevertheless, in the case of our numerical experiments, all five definitions gave a pev median slightly higher for the block_different_mu algorithm than for deflation.

As a check for the choice (53) (54) (55) of the sparsity parameters \( \gamma_j \), we have plotted in figure 6 the decay, as a function of \( \lambda \), of the contributions of each sparse component to the explained variance varopt. As one can see,
the decrease is roughly similar, which indicates that relative size of the $\gamma_j$ is correctly chosen.

Figure 6: Contribution of each component to the explained variance varopt as function of $\lambda$ for the block_same_mu algorithm in the case of 300 samples.

3.2 Sparse versus group-sparse

We illustrate now the effect of imposing sparsity on group of variables rather than on single variables. We use for this the block_different_mu algorithm, which has been found to be the best performer in section 3.1. As shown by Figure 7 it appears that this information, when available, helps greatly the algorithm to retrieve the sparsity structure of the underlying loadings.

Figure 7: True positive rates (dotted lines) and false positive rates (full lines) for each sparse loading versus reduced sparsity parameter $\lambda$. Left: scalar variables, right: group variables.
4 How to define the explained variance associated with non orthogonal components

In unconstrained PCA, the variance explained by $m$ components $Y = AZ$ is given by (5), which rewrites with the block notations:

$$\text{var}Y = \|Y\|^2_F .$$

This is perfect as long as the components $y_j$ are orthogonal. But sparse PCA algorithms generate usually non orthogonal components, and it is known that the use of (61) can lead to overestimate the explained variance, as shown in section 4.2 below. To the best knowledge of the authors, there is no statistical definition of the variance explained by a block of non orthogonal components $Y$. So the problem of defining the variance $\text{var}Y$ in that case arises.

Two definitions have been proposed in the literature. In 2006, Zou et al. [18] introduced the (order dependent) adjusted variance, as the sum of the additional variances explained by each new component; in 2008, Shen et al. [14] introduced an (order independent) total variance, depending only on the subspace spanned by the components. Little is known on the mathematical properties of these definition, except that the total variance is bounded by the variance $\|A\|^2_F$ of the data [14, Theorem 1 p.1021]. In particular, it is not known whether or not these definitions ensure a diminution of the explained variance with respect to unconstrained PCA, and if they coincide with (61) when $Y$ is orthogonal.

So we perform in this section a quite systematic search for possible definitions for the explained variance $\text{var}Y$, under the constraint that $\text{var}Y$ satisfies a set of statistically reasonable necessary conditions. This will result in five (including adjusted and total variance) different definitions of $\text{var}Y$.

Let $Y$ be a block of components associated to a block $Z$ of loadings in the case of linearly independent but possibly non orthogonal components and/or loadings:

$$Y = AZ \in \mathbb{R}^{n \times m}, \quad Z \in \mathbb{R}^{p \times m}, \quad \text{rank}Y = \text{rank}Z = m$$

where the number $m$ of loadings and components satisfies:

$$m \leq \text{rank}A \overset{\text{def}}{=} r .$$

As it will turn out, the unit norm constraint on the $z_j$’s will not always be necessary, so we shall add it only where required. We want to define $\text{var}Y$ in such a way that:
• **property 1**: it reduces to \( \text{var} A \) for a full PCA, where the optimal loadings \( Z \) are the \( r \)-first (unit norm) right singular vectors \( [v_1 \ldots v_r] \) defined in (2). In this case, \( \text{var} Y \) is unambiguously defined as the sum of the variances of the principal components \( Y = A[v_1 \ldots v_r] \), so that:

\[
(64) \quad \text{var} A \overset{\text{def}}{=} \| A \|_F^2 = \sigma_1^2 + \cdots + \sigma_r^2 = \| A[v_1 \ldots v_r] \|_F^2 = \| Y \|_F^2 = \text{var} Y .
\]

• **property 2**: for a given number \( m \) of loadings, the explained variance \( \text{var} Y \) is smaller than the variance explained by the first \( m \) right singular vectors, that is \( \sigma_1^2 + \cdots + \sigma_m^2 \). This is a desirable property, as it will allow to quantify the drop in explained variance with respect to PCA induced by using sparse loading, and will help to make a decision in the trade-off “explained variance versus sparsity”.

• **property 3**: when the components \( Y \) happen to be orthogonal, this explained variance has to coincide with the common sense statistical formula for the variance of a block of independent variables:

\[
(65) \quad \text{var} Y = \sum_{j=1}^{m} \| y_j \|^2 = \| Y \|_F^2 .
\]

We complement now definition (64) of \( \text{var} A \) by an equivalent vector space definition. We denote by:

\[
(66) \quad P_Z = Z (Z^T Z)^{-1} Z^T
\]

the projection operator on the subspace of \( \mathbb{R}^{|p|} \) spanned by the loadings \( Z \), and notice that the space spanned by the loadings \( Z = [v_1 \ldots v_r] \) corresponding to a full PCA is the orthogonal of the kernel of \( A \). Hence

\[
(67) \quad A P_{[v_1 \ldots v_r]} = A ,
\]

and we deduce from (64) a *subspace definition* for \( \text{var} A \):

\[
(68) \quad \text{var} A = \| A P_{[v_1 \ldots v_r]} \|_F^2 .
\]

Note that with this definition, \( \text{var} A \) depends only of the *subspace* spanned by \( [v_1 \ldots v_r] \), so the normalization of loadings \( v_j \) is not required.

We can now start from either (64) or (68) to define the variance explained by the components \( Y = A Z \) associated to any block \( Z \) of \( m \leq r \) linearly independent loading vectors.
4.1 Subspace variance

We generalize in this section formula (68) for $\text{var}_A$, and define, when $Z$ satisfies (62), the *subspace variance* of $Y = AZ$ by:

\[(69) \quad \text{var}_{\text{subsp}} Y \overset{\text{def}}{=} \|A P_Z\|^2_F = \|AZ(Z^TZ)^{-1}Z^T\|^2_F,
\]

where we have used formula (66) for the projection operator $P_Z$. This shows that $\text{var}_{\text{subsp}} Y$ coincides with the total variance explained by $Y$ introduced by Shen and Huang in [14, section 2.3 p. 1021].

Note that this definition is independant of the magnitude of the loading vectors, as mentioned at the beginning of section 4. Of course, we will still continue to represent loadings by unit norm vectors - but this is here only a convenience. The trace formulation of the Frobenius norm gives:

\[(70) \quad \text{var}_{\text{subsp}} Y = \text{tr}\{Z(Z^TZ)^{-1}Z^T A^T A Z (Z^TZ)^{-1}Z^T\} = \text{tr}\{Z(Z^TZ)^{-1}Z^T A^T A Z (Z^TZ)^{-1}\} \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \|A\|^2_F,
\]

where we have used the cyclic invariance of the trace to derive the second equality.

**Lemma 4.1** Let $Z$ satisfy (62). Then the subspace variance of $Y = AZ$ satisfies:

\[(71) \quad \text{var}_{\text{subsp}} Y = \text{tr}\{Y^T Y (Z^TZ)^{-1}\} \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \|A\|^2_F,
\]

and:

\[(72) \quad \text{var}_{\text{subsp}} Y = \sigma_1^2 + \cdots + \sigma_m^2 \iff \begin{cases} \text{span}Y = \text{span}[u_1 \ldots u_m], \\ \text{span}Z = \text{span}[v_1 \ldots v_m], \end{cases}
\]

so that $\text{var}_{\text{subsp}} Y$ satisfies properties 1 and 2.

**Proof:** $\text{var}_{\text{subsp}} Y$ satisfies property 1 by construction, and property 2 results from (71), which together with (72) follows immediately from the properties of the generalized Rayleigh quotient $\text{tr}\{Z^TA^T A Z (Z^TZ)^{-1}\}$ recalled in Theorem 7.1 in section 7.1 of the Appendix.

However, when the components happen to be orthogonal, $Y^T Y$ is diagonal, no simplification occurs in (71), but the following property holds:
Lemma 4.2 Let $Y = AZ$ be a block of $m$ orthogonal components associated to unit norm loadings $Z$. Then:

\[(73) \quad \|Y\|_F^2 \leq \text{var}_{\text{subsp}} Y \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \|A\|_F^2.\]

**Proof:** see section 7.4 of the Appendix. \qed

This shows that the subspace variance misses to satisfy property 3: it overestimates the variance when the components are orthogonal.

Also, when the loadings $Z$ are orthogonal, (71) shows that $\text{var}_{\text{subsp}} Y = \|Y\|_F^2$, but this is again not satisfying from a statistical point of view as now the components $Y$ are generally not orthogonal!

So we explore in the next section another road in the hope of being able to comply with all properties 1, 2 and 3.

### 4.2 Adjusted, optimal and normalized variances

We start in this section from the statistical definition (64). A natural generalization would be:

\[(74) \quad \text{var} Y \overset{2}{=} \|A[z_1 \ldots z_m]\|_F^2 = \|AZ\|_F^2 = \|Y\|_F^2 = \text{tr}\{Y^TY\}.\]

This tentative definition makes sense only if the magnitude of the individual loading vectors if fixed! Hence it has to be used together with the normalization constraint:

\[(75) \quad \|z_j\| = 1, \quad j = 1 \ldots m.\]

This is the current practice in PCA, where the loadings coincide with right singular vectors:

\[(76) \quad Z = [v_1 \ldots v_m],\]

in which case the tentative definition (74) gives:

\[(77) \quad \text{var} Y = \|A[v_1 \ldots v_m]\|_F^2 = \sigma_1^2 + \cdots + \sigma_m^2 \leq \sigma_1^2 + \cdots + \sigma_r^2 = \|A\|_F^2,\]

which corresponds to the upper bound required in property 2.

In the general case of possibly non orthogonal loadings which satisfy only (62) (75), property 2 is not ensured anymore, as many authors have pointed out. For example, consider a matrix $A$ with three singular values $3, 2, 1,
and chose for $Z$ two linearly independant unit vectors close to the first right singular vector $v_1$. Then definition (74) gives:

$$\text{var} Y = \| AZ \|_F^2 = \| Az_1 \|_2^2 + \| Az_2 \|_2^2 \simeq 18 > 9 + 4 + 1 = \| A \|_F^2.$$

This contradicts both properties 1 and 2, which makes (74) inadequate as a general definition of the explained variance.

However, from a statistical point of view, this definition continues to make perfect sense for the explained variance as long as the components are orthogonal, without pointing necessarily in the direction of left singular vectors: the components correspond then to a block of independant variables, whose total variance is defined by (74).

Hence a natural way to eliminate the redundancy caused by the orthogonality default of the components $Y$ and to satisfy property 3 is to:

1. choose an orthogonal basis $X$ of the subspace spanned by the components:

$$X^T X = I_m \quad \text{span}\{X\} = \text{span}\{Y\}.$$

Let $M$ be the matrix of the coordinates of $Y$ in the chosen $X$ basis:

$$M = X^T Y \quad \iff \quad Y = XM.$$

A reasonable criterion for the choice of the basis $X$ is to require that, loosely speaking, it “points in the direction of the components $Y$”. We shall consider two such choices:

- **QR decomposition of $Y$**: after having ordered the components $y_j$ by decreasing norm, this gives:

$$Y = QR \quad , \quad Q^T Q = I_m \quad , \quad R = \text{upper triangular matrix}.$$

followed by:

$$X = Q \quad , \quad \text{so that} \quad M = R.$$

Because the QR orthogonalization procedure is started with the components of largest norm, the basis $X = Q$ will point in the direction of $Y$ at least for the components of larger norm.
• polar decomposition of $Y$ : this is our preferred choice, as it provides the basis $X$ which “points the best in the directions of $Y$” :

(83) \[ Y = UP, \quad U^TU = I_m, \quad P^T = P \in \mathbb{R}^{m \times m}, \quad P \geq 0, \]

followed by :

(84) \[ X = U = Y(Y^TY)^{-1/2}, \quad M = P = (Y^TY)^{1/2}, \]

where we have used the hypothesis [62] that the components $Y$ are linearly independant.

2. associate to $Y$ orthogonal modified components $Y'$ along the $X$ axes, and define $\text{var} Y$ by :

(85) \[ \text{var} Y \overset{\text{def}}{=} \|Y'\|_F^2. \]

We shall consider here two natural choices for the modified components $Y' = (y'_1 \ldots y'_m)$ :

• projection : define $y'_j$ as the projection of $y_j$ on the $j$-th axis of the basis $X$ :

(86) \[ y'_j = \langle y_j, x_j \rangle x_j = m_{j,j} x_j, \quad j = 1 \ldots m. \]

Lemma 4.3 For any orthogonal basis $X$ satisfying (79), the modified components $Y'$ defined by projection (86) satisfy :

(87) \[ \|Y'\|_F^2 = \text{tr}\{\text{diag}^2 M\} \leq \text{var}_{\text{subsp}} Y \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \|A\|_F^2. \]

The proof is given in section [7.5] of the Appendix.

• normalization : choose $y'_j$ in the direction of $x_j$ such that :

(88) \[ y'_j = Az'_j, \quad \text{with} \quad \|z'_j\| = 1, \quad j = 1 \ldots m. \]

By construction $x_j \in \text{span} Y$ - see (79) - and both $Y = AZ$ and $Z$ are made of linearly independant vectors - see (62) - hence :

(89) \[ \forall j = 1 \ldots m, \quad \exists ! t_j \in \text{span} Z \quad \text{such that} \quad x_j = At_j. \]

The unit norm loadings $z'_j$ which satisfy (88) are then given by :

(90) \[ z'_j = \|y'_j\| t_j, \quad j = 1 \ldots m, \]

and the following Lemma holds :
Lemma 4.4 For any orthogonal basis $X$ satisfying (79), the modified components $Y'$ defined by normalization (88) satisfy:

\[
\|Y'\|_F^2 = \sum_{j=1}^{m} 1/\|t_j\|^2 \leq \text{var}_{\text{subsp}} Y \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \|A\|^2_F ,
\]

where the loadings $t_j$'s are defined by (89).

The proof of the Lemma follows immediately from Lemma 4.2 applied to the orthogonal components $Y' = AZ'$.

Notice that when $Y'$ is defined by normalization as above, $\|Y'\|_F^2$ depends solely on the basis $X$, so it is linked to the components $Y$ only by the process (80) used to associate $X$ to $Y$ ! Once this process has been chosen, the loadings $T$ whose existence is asserted by (89) are easily obtained by performing on the loadings $Z$ the same linear combinations which transformed $Y$ into $X$:

\[
Z = TM , \quad \text{to be compared to} \ (80) : \ Y = XM .
\]

Depending on the choices made at steps 1 and 2, formula (85) gives four possible definitions for the explained variance, which all satisfy properties 1 and 3 by construction, and property 2 by virtue of Lemmas 4.3 and 4.4:

**Adjusted variance.** Define $Y'$ by *projection* (86) and $XM$ by *QR-decomposition* (81) (82) of $Y$. Then (85) (87) give:

\[
\text{var}_{\text{proj}}^{QR} Y = \text{tr}\{\text{diag}^2 R\} = \text{tr}\{R^2\} = \langle R^T, R \rangle_F ,
\]

which is the *adjusted variance* introduced by Zou et al. in [18].

**Optimal variance.** Define still $Y'$ by *projection* but $XM$ by the *polar decomposition* $UP$ of $Y$ (83) (84). Formula (85) (87) give now:

\[
\text{var}_{\text{proj}}^{UP} Y = \text{tr}\{\text{diag}^2 P\} = \text{tr}\{\text{diag}^2(Y^TY)^{1/2}\} .
\]

This variance is *optimal* in the sense that, when $Y'$ is defined by projection, it is larger that the variance obtained with any other choice of the basis $X$ (proposition 4.7 below) - in particular larger than the adjusted variance $\text{var}_{\text{proj}}^{QR} Y$. 

25
QR normalized variances. Let now $Y'$ be defined by normalization, and $XM$ by QR decomposition of $Y$. Then (85)-(91) lead to another definition of explained variance:

$$
\text{(95)} \quad \text{var}_{\text{norm}}^{QR} Y = \sum_{j=1}^{m} \frac{1}{\|t_j\|^2} = \text{tr}\{\text{diag}^{-1}(T^TT)\} \quad \text{where} \quad T = ZR^{-1}.
$$

UP normalized variances. With $Y'$ still defined by normalization, but $XM$ by polar decomposition $UP$ of $Y$, formula (85)-(91) define a new explained variance:

$$
\text{(96)} \quad \text{var}_{\text{norm}}^{UP} Y = \sum_{j=1}^{m} \frac{1}{\|t_j\|^2} = \text{tr}\{\text{diag}^{-1}(T^TT)\} \quad \text{where} \quad T = Z(Y^TY)^{-1/2}.
$$

Remark 4.5 There is no natural ordering between the explained variances defined by (87) - projection, and (91) - normalization, as illustrated in Figure 8 for the case of polar decomposition: the two sets of components $Y = [y_1 \ y_2]$ and $\tilde{Y} = [\tilde{y}_1 \ \tilde{y}_2]$ have been chosen such that their polar decomposition produces the same basis $X = [x_1 \ x_2]$, and one sees that:

$$
\text{(97)} \quad \text{var}_{\text{proj}}^{UP} \tilde{Y} \leq \text{var}_{\text{norm}}^{UP} \tilde{Y} = \text{var}_{\text{norm}}^{UP} Y \leq \text{var}_{\text{proj}}^{UP} Y.
$$

Remark 4.6 There is no natural ordering between $\text{var}_{\text{norm}}^{QR}$ and $\text{var}_{\text{norm}}^{UP}$: for components $y_1 \ldots y_m$ such that the basis $x_1 \ldots x_m$ associated by QR-decomposition coincides with the $m$-first left singular vectors $u_1 \ldots u_m$ of $A$, one has, according to Lemma 4.4:

$$
\text{(98)} \quad \text{var}_{\text{norm}}^{QR} Y = \sigma_1^2 + \cdots + \sigma_m^2 \geq \text{var}_{\text{norm}}^{UP} Y,
$$

with a strict inequality as soon as $y_1 \ldots y_m$ and $u_1 \ldots u_m$ don't coincide. Similarly, if components $Y$ are such that the basis $x_1 \ldots x_m$ associated by polar decomposition coincides with the $m$-first left singular vectors $u_1 \ldots u_m$ of $A$, one has:

$$
\text{(99)} \quad \text{var}_{\text{norm}}^{UP} Y = \sigma_1^2 + \cdots + \sigma_m^2 \geq \text{var}_{\text{norm}}^{QR} Y,
$$

with a strict inequality as soon as $y_1 \ldots y_m$ and $u_1 \ldots u_m$ don't coincide.
The next proposition summarize the properties of the various definitions:

**Proposition 4.7** Let $Y = AZ$ be components associated to the loadings $Z$, $\sigma_1 \ldots \sigma_m$ and $v_1 \ldots v_m$ be the $m$ first singular values and right singular vectors of $A$, and suppose that (62) hold.

1. the subspace variance $\text{var}_{\text{subsp}}$ of Shen and Huang [14] satisfies:
   
   $\text{(100)} \quad \text{var}_{\text{subsp}} Y \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \|A\|_F^2$,

   $\text{(101)} \quad \text{var}_{\text{subsp}} Y = \sigma_1^2 + \cdots + \sigma_m^2 \iff \text{span } Z = \text{span } \{v_1 \ldots v_m\}$,

   so it satisfies properties 1 and 2. But when the components $Y$ are orthogonal, one has only:

   $\text{(102)} \quad \|Y\|_F^2 \leq \text{var}_{\text{subsp}} Y$,

   so $\text{var}_{\text{subsp}} Y$ does not satisfy property 3.

2. the adjusted variance $\text{var}_{\text{proj}}^{QR}$ of Zou et al. [18] and the optimal variance $\text{var}_{\text{proj}}^{UP}$ defined by projection satisfy:

   $\text{(103)} \quad \text{var}_{\text{proj}}^{QR} Y \leq \text{var}_{\text{proj}}^{UP} Y \leq \text{var}_{\text{subsp}} Y \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \|A\|_F^2$,

   and both satisfy properties 1, 2 and 3.
3. The normalized variances \( \text{var}_{\text{norm}}^{QR} \) (95) and \( \text{var}_{\text{norm}}^{UP} \) (96) satisfy:

\[
(104) \quad \text{var}_{\text{norm}}^{QR} Y \leq \text{var}_{\text{subsp}} Y \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \|A\|_F^2,
\]

\[
(105) \quad \text{var}_{\text{norm}}^{UP} Y \leq \text{var}_{\text{subsp}} Y \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \|A\|_F^2,
\]

and both satisfy properties 1, 2 and 3. There is no natural order between \( \text{var}_{\text{norm}}^{QR} \) and \( \text{var}_{\text{norm}}^{UP} \).

4. There is no natural order between \( \text{var}_{\text{proj}}^{QR} \) and \( \text{var}_{\text{proj}}^{UP} \) on one side, and \( \text{var}_{\text{norm}}^{QR} \) and \( \text{var}_{\text{norm}}^{UP} \) on the other side.

5. For any of the four last definitions \( \text{var}_{\text{proj}}^{QR} Y \), \( \text{var}_{\text{proj}}^{UP} Y \), \( \text{var}_{\text{norm}}^{QR} Y \), \( \text{var}_{\text{norm}}^{UP} Y \) of \( \text{var} Y \) one has:

\[
(106) \quad \text{var} Y = \sigma_1^2 + \cdots + \sigma_m^2 \implies \text{span} Z = \text{span}\{v_1 \ldots v_m\},
\]

\textbf{Proof:} Point one summarizes the results of Lemma 4.1 and 4.2, and of theorem 7.1 recalled in section 7.1 of the Appendix.

Next we prove the left inequality of (103). For a given \( Y \in \mathbb{R}^{m \times n} \) we want to prove that the function \( h : X \mapsto \sum_{i=1}^{m} (y_j, x_j)^2 \) is maximum at \( X = U = \text{polar} \) over all \( X \in S_m^n \). The maximizer \( \hat{X} \) is necessarily a fixed point of the iterative process \( X_{k+1} = \text{polar} \nabla_X h(X_k) \) (see [7, page 531] or Algorithm 1 in section 7.2 of the Appendix), hence \( \hat{X} = \text{polar} \nabla_X h(\hat{X}) \). But \( \nabla_X h(X) = 2Y \) so \( \text{polar} \nabla_X h(\hat{X}) = \text{polar}(2Y) = U \) given by (83). The remaining inequalities in (103) follow then immediately from Lemma 4.3 applied with the orthogonal basis \( \hat{X} = U \) produced by the polar decomposition of \( Y \).

Then point 3 follows immediately from lemma 4.4 applied with the choices \( XM = QR \) (for the proof of (104)) or \( XM = UP \) (for the proof of (105)). Counter examples for point 4 have been illustrated in remark 4.5, and finally, point 5 follows from points 1, 2 and 3.

In conclusion, this analysis suggests to use \( \text{var}_{\text{proj}}^{UP} Y \) or \( \text{var}_{\text{norm}}^{UP} Y \) as measures of explained variance, as they are the only ones which satisfy properties 1, 2 and 3 and are order independent.

5 Numerical comparison of explained variance definitions

We compare in this section the five definitions of \( \text{var} Y \) of section 4 on the sets of (non orthogonal) components \( Y \) obtained in section 3 on the comparison
of algorithms. We display the dimensionless proportion of explained variance (pev) defined by:

\[
0 \leq \text{pev} = \frac{\text{var}Y}{\|A\|_F^2} \leq \frac{(\sigma_1^2 + \cdots + \sigma_m^2)}{\|A\|_F^2},
\]

where the right inequality follows from Proposition 4.7 with equality holding when no sparsity is required. Definition (85) of varY shows that each component \(y_j\) contributes to the pev in the amount of

\[
\theta_j = \frac{\|y_j\|^2}{\|A\|_F^2}, \quad \sum_{i=1}^{m} \theta_j = \text{pev}.
\]

5.1 Comparison of explained variances

We compare now the five definitions for the explained variance varY discussed in section 4. We show first in Figure 9, for each \(\lambda\) and for each definition of varY, the mean values over the realizations of A of the pev defined by (107). The figure shows that these mean pev’s are in the same order for all \(\lambda\) and all algorithms:

\[
\text{subspVar} \geq \text{optVar} \geq \text{adjVar} \geq \text{QRnormVar} \geq \text{UPnormVar}.
\]

![Figure 9: Comparison of the mean pev’s (proportion of explained variance) as function of reduced sparsity parameter \(\lambda\) for the three algorithms.](image)
The two first inequalities, and the fact the mean values of QRnormVar and UPnormVar are smaller than subspVar, have been proved in proposition 4.7. But the good surprise is that there seems to be an apparent order between the mean values of the normalized variances between themselves and with respect to the projected variances. As one can see in table 1 however, this order fails to hold for some realizations of $A$, namely in less than 10% of cases for QRnormVar, and less than 3% of cases for UPnormVar.

|        | subspVar | optVar | adjVar | QRnormVar | UPnormVar |
|--------|----------|--------|--------|-----------|-----------|
| subspVar | 100.00   | 100.00 | 100.00 | 100.00    | 100.00    |
| optVar  | 100.00   | 100.00 | 98.67  | 99.23     | 99.23     |
| adjVar  | 100.00   | 89.58  | 97.15  |           |           |
| QRnormVar | 100.00  | 99.60  |        |           |           |
| UPnormVar |        | 100.00 | 99.60  |           |           |

Table 1: The entry of the table on line $i$ and column $j$ gives the percentage of realizations of $A$ for which $pev_i \geq pev_j$.

When it comes to real data, the variability of the explained variance is an important feature, as only one realization is available. As it appears in figure 10, subspVar and optVar exhibit the smallest dispersion. This leads us to select the optimal variance optVar as definition of choice for explained variance, as it exhibits the smallest dispersion among definitions which satisfy properties 1-3 and are order independent.
Figure 10: Boxplots of the five pev (proportion of explained variance) obtained for $\lambda = 0.2$ with the block algorithm with different mu’s.

### 5.2 Ranking properties of explained variances

The proportions of explained variance $\text{pev}_i, i = 1 \ldots 5$ defined by (107) are meant to be used for the ranking of algorithms, so it is important to figure out whether or not different $\text{pev}_i$ and $\text{pev}_j$ will rank in the same order the components $Y_P$ and $Y_Q$ obtained by applying algorithms $P$ and $Q$ with sparsity parameter $\lambda$ to the data matrix $A$. There are 3 algorithms, 50 values of $\lambda$ and 100 realizations of $A$, and hence 15000 couples of components to be tested. Among these couples, we may consider as $\epsilon$-distinguishable from the point of view of our explained variances those for which

$$|\text{pev}_i(Y_P) - \text{pev}_i(Y_Q)| \geq \epsilon \quad \text{forall} \quad i = 1 \ldots 5$$

for some $\epsilon \geq 0$. Table 2 shows the percentage of cases where $\text{pev}_i$ and $\text{pev}_j$ rank identically components $Y_P$ and $Y_Q$ among all $\epsilon$-distinguishable couples. The good news here is that the ranking is essentially independent of the explained variance definition as soon as one considers that differences in proportion of explained variance under $10^{-2}$ are not significative.
| subspVar | optVar | adjVar | QRnormVar | UPnormVar |
|----------|--------|--------|-----------|-----------|
| subspVar | 90.52  | 73.55  | 65.23     | 64.55     |
| optVar   | 80.35  | 71.41  | 70.70     |           |
| adjVar   | 87.15  |        | 88.77     |           |
| QRnormVar|        |        | 88.19     |           |
| UPnormVar|        |        |           |           |

| subspVar | optVar | adjVar | QRnormVar | UPnormVar |
|----------|--------|--------|-----------|-----------|
| subspVar | 99.10  | 91.04  | 84.49     | 89.78     |
| optVar   | 91.94  |        | 85.40     | 90.68     |
| adjVar   |        | 93.17  |           | 98.74     |
| QRnormVar|        |        | 93.98     |           |
| UPnormVar|        |        |           |           |

| subspVar | optVar | adjVar | QRnormVar | UPnormVar |
|----------|--------|--------|-----------|-----------|
| subspVar | 100.00 | 100.00 | 99.93     | 100.00    |
| optVar   | 100.00 |        | 99.93     | 100.00    |
| adjVar   |        | 99.93  |           | 100.00    |
| QRnormVar|        |        | 99.93     |           |
| UPnormVar|        |        |           |           |

Table 2: The entry of each table on line $i$ and column $j$ gives the percentage of $\epsilon$-distinguishable couples $Y_P, Y_Q$ which are ranked identically by $\text{pev}_i$ and $\text{pev}_j$. Top : $\epsilon = 0$, middle : $\epsilon = 10^{-3}$, bottom : $\epsilon = 10^{-2}$.

### 6 Conclusion

We have proposed a new block approach for the construction of group-sparse PCA, which reduces to the maximization a convex function over a Stiefel manifold. The resulting Group-Sparse Block PCA algorithm generalizes one algorithm of [7]. The numerical results on simulated data with four group-sparse underlying loadings show that:

- group-sparse block PCA is more effective than deflation in retrieving the sparse structure of the underlying loading vectors,
- group-sparse block PCA produces a slightly higher level of optimal (explained) variance,
- the group information greatly helps the algorithm to retrieve the underlying group-sparsity structure.
Then we have performed a mathematical study of five tentative definitions (two existing and three new ones) of the explained variance for sets of non orthogonal components, such as those produced by sparse ACP. We prove that four of five definitions pass all tests, but that \textit{subspace variance} \cite{13} fails for one. However, numerical results show that all five definitions rank sets of components essentially in the same order, provided the differences in proportion of explained variances are larger than 0.01. \textit{Optimal variance} \cite{94}, which exhibits the smallest dispersion, is order independant, and is larger than \textit{adjusted variance} \cite{15}, is a definition of choice for explained variance.

7 Appendix

7.1 Generalized Rayleigh quotient

We recall here the properties of the generalized Rayleigh quotient

\begin{equation}
\text{tr}\{(Z^T A^T AZ)(Z^T Z)^{-1}\}
\end{equation}

associated to a data matrix \(A \in \mathbb{R}^{n \times |p|}\) and a loading matrix \(Z \in |p| \times m\):

\textbf{Theorem 7.1} Let the loadings \(Z\) satisfy :

\begin{equation}
Z = [z_1 \ldots z_m] \in \mathbb{R}^{|p| \times m}, \quad \text{rank } Z = m \leq \text{rank } A \overset{\text{def}}{=} r.
\end{equation}

Then the generalized Rayleigh quotient \((111)\) satisfies :

\begin{equation}
\text{tr}\{(Z^T A^T AZ)(Z^T Z)^{-1}\} \leq \sigma_1^2 + \cdots + \sigma_m^2 \leq \text{var } A = \|A\|_F^2,
\end{equation}

and the left inequality becomes an equality if and only if :

\begin{equation}
\text{span } Z = \text{span}\{v_1 \ldots v_m\},
\end{equation}

where \(v_1, \ldots v_m\) are the \(m\) first right singular vectors of \(A\).

\textbf{Proof:} it can be found, for example, in \cite[Proposition 2.1.1]{2}. We recall it here with our notations for the ease of the reader. We suppose that \(\sigma_m > \sigma_{m+1}\), but the result remains true without this hypothesis. The projection operator \(P_Z\) - and hence the explained variance \(\text{var}_{\text{subsp}} Y\) - is unchanged if one replaces the given block \(Z\) of linearly independant vectors by a block of
orthonormal vectors which spans the same subspace. So without restriction, we can suppose that :

\[(115)\qquad Z^T Z = I_m ,\]

Let then \( M = W^T Z \) be the \(|p| \times m\) matrix whose \(j\)th column is made of the coefficients of \(z_j\) on the orthogonal \(|p| \times |p|\) matrix \(W\) of the right singular vectors of \(A\) as defined in \((2)\). Then \( M^T M = Z^T W W^T Z = I_m\), so that :

\[(116)\quad \forall j = 1 \ldots m : \sum_{i=1}^{|p|} m_{ij}^2 = 1 \quad \text{and} \quad \forall i = 1 \ldots |p| : \sum_{j=1}^{m} m_{ij}^2 \leq 1 .\]

The loadings \(Z\) are orthogonal - c.f. \((115)\) - so \((71)\) shows that \(\text{var}_{\text{subsp}} Y\) can be computed by \((74)\) :

\[
\text{var}_{\text{subsp}} Y = \text{tr}(Z^T A^T A Z) = \text{tr}(M^T W^T A^T A W M) = \text{tr}(M^T \Sigma^T \Sigma M) = \sum_{i=1}^{|p|} \sigma_i^2 \sum_{j=1\ldots m} m_{ij}^2 .
\]

\[
= \sum_{j=1\ldots m} \left( \sum_{i=1}^{|p|} \sigma_i^2 m_{ij}^2 + \sigma_m^2 - \sigma_m^2 \sum_{i=1}^{|p|} m_{ij}^2 \right) \quad \text{(use \((116)\) left)}
\]

\[
= \sum_{j=1\ldots m} \left( \sigma_m^2 + \sum_{i=1}^m (\sigma_i^2 - \sigma_m^2)m_{ij}^2 + \sum_{i=m+1}^{|p|} (\sigma_i^2 - \sigma_m^2)m_{ij}^2 \right)
\]

\[(117)\quad = \sum_{i=1}^m \sigma_i^2 + \sum_{i=1}^m (\sigma_m^2 - \sigma_i^2) \left( 1 - \sum_{j=1\ldots m} m_{ij}^2 \right) + \sum_{j=1}^m \sum_{i=m+1}^{|p|} (\sigma_i^2 - \sigma_m^2)m_{ij}^2 .
\]

The singular values are numbered in decreasing order, so in \((117)\) the second term (use also the right part of \((116)\)) and the third term are negative. This ends the proof of the right inequality in \((105)\). Equality holds if and only if these two terms vanish, which can happen only if \(m_{ij} = 0 \forall i = m + 1 \ldots |p|\) (third term). This in turn implies that the upper \(m \times m\) block of \(M\) is orthogonal, and the second term vanishes too. Hence the loadings \(Z\) are combinations of the \(m\) first singular vectors of \(A\) only.
7.2 Maximization on a manifold

We recall here the algorithm proposed by Journé et al. [7, Algorithm 1 page 526] for the maximization of a convex function $f$ on a compact set (manifold) $M$ of a finite dimensional space $E$. We suppose that $E$ has been identified to its dual, and denote by $\nabla^s f(x)$ one subgradient of $f$ at $x \in E$.

**Algorithm 1**

**input**: $x_0 \in M$

**output**: $x_n$ (approximate solution)

```
begin
    0 ←− k
    repeat
        $x_{k+1} \in \arg \max_{y \in M} \{f(x_k) + \langle \nabla^s f(x_k), y - x_k \rangle\}$
        $k ←− k + 1$
    until a stopping criterion is satisfied
end
```

This algorithm is applied with $E = \mathbb{R}^{n \times m}$ and $M = S^m_n$ (Stiefel variety made of $m$ orthogonal unit vectors of $\mathbb{R}^n$) in section 2.1 and 2.2.

7.3 Proof of proposition 2.1

We give first an analytical solution to the inner maximization problem in (37): we show that

\[
\forall X \in S^m_n, \quad \max_{Z \in (\mathcal{B}(p))^m} f_{\text{CL}}^{gs}(X, Z) = F(X) \text{ given by (40)},
\]

which proves (45). We adapt to the case of group variables the approach given in [7] for the case of scalar variables.

So let $X$ be a given point on the Stiefel manifold $S^m_n$. Then:

\[
\begin{align*}
(118) \quad \max_{Z \in (\mathcal{B}(p))^m} f_{\text{CL}}^{gs}(X, Z) &= \max_{\|z_j\| \leq 1, \ j = 1, \ldots, m} \sum_{j=1}^{m} \mu_j^2 \left[ x_j^T A z_j - \gamma_j \|z_j\|_1 \right]_+^2, \\
(119) \quad &= \sum_{j=1}^{m} \mu_j^2 \max_{\|z_j\| \leq 1} \left[ x_j^T A z_j - \gamma_j \|z_j\|_1 \right]_+^2, \\
(120) \quad &= \sum_{j=1}^{m} \mu_j^2 \max_{\|z_j\| \leq 1} \left[ x_j^T A z_j - \gamma_j \|z_j\|_1 \right]_+^2.
\end{align*}
\]

But $t \mapsto [t]_+^2$ is a monotonously increasing function, hence:

\[
\begin{align*}
(121) \quad \max_{Z \in (\mathcal{B}(p))^m} f_{\text{CL}}^{gs}(X, Z) &= \sum_{j=1}^{m} \mu_j^2 \left[ \max_{\|z_j\| \leq 1} (x_j^T A z_j - \gamma_j \|z_j\|_1) \right]_+^2.
\end{align*}
\]
The max in the right-hand side of (121) is certainly positive, as \( z_j = 0 \) belongs to the admissible set \( \{ z \mid \| z \| \leq 1 \} \), and (121) becomes:

\[
\max_{Z \in \mathcal{B}_m} f_{C_L}^{gs}(X, Z) = \sum_{j=1}^{m} \mu_j \left( \max_{\|z_j\| \leq 1} (x_j^T A z_j - \gamma_j \| z_j \|_1) \right)^2,
\]

Hence the inner maximization problem (119) reduces to the solution of \( m \) problems of the same form. So we drop the index \( j \), and consider now, for a given \( x \) in the unit sphere of \( \mathbb{R}^n \), the resolution of the optimization problem:

\[
\begin{align*}
z^* & = \arg \max_{\|z\| \leq 1} (x^T A z - \gamma \| z \|_1) \\
& = \arg \max_{\|z\|_2 \leq \ldots \leq \|z_p\| \leq 1} \left( x^T a_i z_i - \gamma \| z_i \| \right),
\end{align*}
\]

where the \( z_i \in \mathbb{R}^{p_i} \) are the loadings associated to each group variable. We introduce the polar decomposition (cf (41)) of \( z_i \) in \( \mathbb{R}^{p_i} \):

\[
z_i = v_i \beta_i, \quad \text{with} \quad \| v_i \| = 1, \quad \beta_i \geq 0.
\]

and replace the search for \( z^* \) by that for \( v_i^*, \beta_i^*, i = 1 \ldots p \). Then equation (124) becomes, using (43):

\[
\begin{align*}
(v_i^*, \beta_i^*, i = 1 \ldots p) &= \arg \max_{\sum_{i=1}^{p} \beta_i^2 \leq 1} \sum_{i=1}^{p} \max_{\|v_i\| = 1} \left( \alpha_i \beta_i u_i^t v_i - \gamma \beta_i \right). \\
& \sum_{i=1}^{p} \beta_i^2 \leq 1 \quad \beta_i \geq 0, \quad i = 1 \ldots p.
\end{align*}
\]

The argument of the last maximum is obviously:

\[
v_i^* = u_i, \quad i = 1 \ldots p,
\]

and (126) reduces to:

\[
\begin{align*}
(\beta_i^*, i = 1 \ldots p) &= \arg \max_{\sum_{i=1}^{p} \beta_i^2 \leq 1} \sum_{i=1}^{p} \max_{\beta_i \geq 0, \beta_i = 1} \left( \alpha_i - \gamma \right) \beta_i, \\
& \sum_{i=1}^{p} \beta_i^2 \leq 1 \quad \beta_i \geq 0, \quad i = 1 \ldots p
\end{align*}
\]

Define:

\[
I_+ = \{ i = 1 \ldots p \mid \alpha_i - \gamma > 0 \}.
\]
• either : \( I_+ = \emptyset \), and :

\[
\beta^* = 0
\]

is a trivial solution of (128) - but not necessarily unique if \( \alpha_i - \gamma = 0 \) for some \( i \).

• or : \( I_+ \neq \emptyset \). We check first that in this case :

\[
\beta^*_i = 0 \quad \forall i \notin I_+.
\]

For that purpose, suppose that \( \beta^*_i > 0 \) for some \( \ell \notin I_+ \), and let \( k \) be an index of \( I_+ \). One can define \( \tilde{\beta}^* \) by \( \tilde{\beta}^*_i = \beta^*_i \) for \( i \neq k, \ell \), \( \tilde{\beta}^*_\ell = 0 \), and \( \tilde{\beta}^*_k > \beta^*_k \) such that \( \|\tilde{\beta}^*\| = \|\beta^*\| \leq 1 \). Then :

\[
\begin{align*}
(\alpha_\ell - \gamma)\beta^*_\ell &\leq 0 = (\alpha_\ell - \gamma)\tilde{\beta}^*_\ell, \\
(\alpha_k - \gamma)\beta^*_k &< (\alpha_k - \gamma)\tilde{\beta}^*_k,
\end{align*}
\]

which contradicts the fact that \( \beta^* \) is a maximizer, and ends the proof of (131).

We can now restrict the search to the \((\beta^*_i, i \in I_+)\), so (128) simplifies to :

\[
(132) \quad (\beta^*_i, i \in I_+) = \arg \max \quad \sum_{i \in I_+} (\alpha_i - \gamma)\beta_i, \\
\quad \text{subject to} \quad \beta_i \geq 0, \quad i \in I_+ \quad \text{and} \quad \sum_{i \in I_+} \beta_i^2 \leq 1
\]

\[
(133) \quad = \arg \max \quad \sum_{i \in I_+} (\alpha_i - \gamma)\beta_i, \\
\quad \text{subject to} \quad \sum_{i \in I_+} \beta_i^2 \leq 1
\]

where the last equality holds because the coefficients \( \alpha_i - \gamma \) of \( \beta_i \) are positive for \( i \in I_+ \). Hence the solution \( \beta^* \) of (128) is given, when \( I_+ \neq \emptyset \), by :

\[
(134) \quad \beta^*_i = \frac{[\alpha_i - \gamma]_+}{\left(\sum_{i=1...p} [\alpha_i - \gamma]_+^2\right)^{1/2}}, \quad i = 1 \ldots p,
\]

Returning to the \( z \) unknowns one obtains, using (125) (127) (130) (134) :

\[
(135) \quad z^* = \begin{cases} 
0 & \text{if } I_+ = \emptyset, \\
(z^*_i = u_i\beta^*_i; i = 1 \ldots, p) & \text{if } I_+ \neq \emptyset,
\end{cases}
\]

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and in both cases the maximum of the optimization problem (123) is given by:

\[
\max_{\|z\|_1 \leq 1} (x^T A z - \gamma \|z\|_1) = \left( \sum_{i=1}^{p} [\alpha_i - \gamma]_+^2 \right)^{1/2}.
\]

Reintroducing the \(j\) indices, the solution of the inner maximization problem (119), for a given \(X \in S_m^n\), is, using its reformulation (122) together with (135), (136) and the notation \(t_j \in \mathbb{R}^{\|p\|}\) defined by (44):

\[
\forall j = 1 \ldots m, \quad z_j^* = \begin{cases} 0 & \text{if } t_j = 0, \\ t_j/\|t_j\| & \text{if } t_j \neq 0, \end{cases}
\]

\[
\max_{Z \in (S_{\|p\|})^m} f_{CL}^g(X, Z) = \sum_{j=1 \ldots m} \mu_j^2 \|t_j\|^2 = F(X).
\]

The last equation proves (40), and hence part 1 of the theorem. Then (137) gives (46) when \(X\) is a solution \(X^*\) of (45), and part 2 is proved.

We prove now point 3 of the proposition: let the sparsity parameters \(\gamma_j\) satisfy (47). Hence there exists \(\ell \in 1 \ldots m\) and \(k \in 1 \ldots p\) such that:

\[
\gamma_\ell < \|a_k\|_2 = \|a_k^\ell\|_2.
\]

By definition of the matrix norm \(\|\cdot\|_2\), there exists \(X \in S_m^n\) such that \(x_\ell\) satisfies:

\[
\gamma_\ell < \|a_k^\ell x_\ell\| = \alpha_{k\ell}.
\]

Then (44) gives:

\[
\|t_\ell\|^2 \geq (\alpha_{k\ell} - \gamma_\ell)^2 > 0 \quad \implies \quad t_\ell \neq 0,
\]

and point 3 is proven.

### 7.4 Proof of Lemma 4.2

Let \(Y = AZ\) be a given such that

\[
\langle y_j, y_k \rangle = 0, \quad j, k = 1 \ldots m, j \neq k, \quad \|z_j\| = 1, \quad j = 1 \ldots m,
\]

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and define $X, T$ by:

$$x_j = y_j / \|y_j\| \quad , \quad t_j = z_j / \|y_j\| \quad , \quad j = 1 \ldots m ,$$

so that:

$$X^T X = I_m .$$

Then on one side one has:

$$\|Y\|_F^2 = \sum_{j=1}^{m} \|y_j\|^2 = \sum_{j=1}^{m} 1/\|t_j\|^2 = \text{tr}\{\text{diag}^{-1}(T^T T)\} ,$$

and on the other side, as $Y$ and $X$ span the same subspace:

$$\text{var}_{subsp} Y = \text{var}_{subsp} X = \text{tr}\{(X^T X)(T^T T)^{-1}\} = \text{tr}\{(T^T T)^{-1}\}$$

The lemma will be proved if we show that:

$$\text{tr}\{\text{diag}^{-1}(T^T T)\} \leq \text{tr}\{(T^T T)^{-1}\} .$$

We use for that an idea taken from [9], and perform a QR-decomposition of $T$. By construction, the diagonal elements of $R$ satisfy:

$$0 < r_{i,i} \leq \|t_i\| .$$

Then:

$$T^T T = R^T Q^T Q R = R^T R ,$$

$$\text{(}T^T T\text{)}^{-1} = (R^T)^{-1} = (R^{-1})^T \text{ ,}$$

where $R^{-1}$ satisfies:

$$R^{-1} = \text{upper triangular matrix} \quad , \quad [R^{-1}]_{i,i} = 1/r_{i,i} .$$

Hence the diagonal element of $(T^T T)^{-1}$ are given by:

$$[\text{(}T^T T\text{)}^{-1}]_{i,i} = \left[ R^{-1}(R^{-1})^T \right]_{i,i}$$

$$= [R^{-1}]_{i,i}^2 + \sum_{j>i} [R^{-1}]_{i,j}^2$$

$$\geq [R^{-1}]_{i,i}^2 = 1/r_{i,i}^2 \geq 1/\|t_i\|^2 .$$

which gives (147) by summation over $i = 1 \ldots m$, and ends the proof. ■
7.5 Proof of Lemma 4.3

Let $E = AS|p|$ be the $n$-dimensional ellipsoid image by $A$ of the unit sphere $S|p| \subset IR|p|$, and:

$\mathcal{E}^X = E \cap \text{span} Y = E \cap \text{span} X$

the $m$-dimensional ellipsoid, trace of $E$ on the subspace spanned both by the given components $Y$ and the chosen basis $X$. By construction one has:

$y_j \in \mathcal{E}^X, \quad j = 1 \ldots m,$

and the modified components $Y'$ defined by projection satisfy, c.f. (86):

$\|y'_j\| = |\langle y_j, x_j \rangle| \leq \nu_j \overset{\text{def}}{=} \max_{y \in \mathcal{E}^X} \langle y, x_j \rangle, \quad j = 1 \ldots m,$

so that:

$\|Y'\|_F^2 \leq \nu_1^2 + \cdots + \nu_m^2.$

We can now "box" the ellipsoid $\mathcal{E}^X$ in the parallelootope $\mathcal{P}^X$ of span$X$ defined by:

$\mathcal{P}^X = \{y \in \text{span} X \mid -\nu_j \leq \langle y, x_j \rangle \leq +\nu_j, \quad j = 1 \ldots m\},$

(see figure 11). By construction, one can draw from each of the $2^m$ vertices of $\mathcal{P}^X$ $m$ orthogonal hyperplanes tangent to the ellipsoid $\mathcal{E}^X$, which implies that they are all on the orthoptic or Cartan sphere of the ellipsoid, whose radius is known to be the sum of the squares of the semi-principal axes $\sigma_j^X, j = 1 \ldots m$ of $\mathcal{E}^X$ (see for example the textbook [16]).

Hence:

$\nu_1^2 + \cdots + \nu_m^2 = (\sigma_1^X)^2 + \cdots + (\sigma_m^X)^2.$

Let then $y_1^X \ldots y_m^X$ be vectors whose extremity are points of $\mathcal{E}^X$ located on its principal axes, so that:

$\|y_j^X\| = \sigma_j^X, \quad j = 1 \ldots m, \quad \langle y_i^X, y_j^X \rangle = 0, \quad i, j = 1 \ldots m, i \neq j.$

Then Lemma 4.2 applied to $Y = Y^X$ gives:

$(\sigma_1^X)^2 + \cdots + (\sigma_m^X)^2 = \|Y^X\|^2 \leq \text{var}_{\text{subsp}} Y^X \leq \sigma_1^2 + \cdots + \sigma_m^2.$

Combining inequalities (156) (158) (160) gives the expected result (87) \[\square\]
Figure 11: Illustration of the upper bound to $\|Y''\|^2_F$ in $\text{span}Y$ when $Y''$ is defined by projection.

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