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► **To cite this version:**

Hugo Brehier, Arnaud Breloy, Mohammed Nabil El Korso, Sandeep Kumar. ROBUST AND GLOBALLY SPARSE PCA VIA MAJORIZATION-MINIMIZATION AND VARIABLE SPLITTING. ICASSP 2023 - 2023 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), Jun 2023, Rhodes Island, France. 10.1109/ICASSP49357.2023.10094882 . hal-04399125

**HAL Id: hal-04399125**

**<https://hal.science/hal-04399125>**

Submitted on 17 Jan 2024

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# ROBUST AND GLOBALLY SPARSE PCA VIA MAJORIZATION-MINIMIZATION AND VARIABLE SPLITTING

Hugo Brehier, Arnaud Breloy, Mohammed Nabil El Korso, Sandeep Kumar

## ABSTRACT

This paper addresses the problem of robust and sparse PCA. We consider a formulation combining a  $M$ -estimation type robust subspace recovery term and a mixed norm that promotes structured sparsity in the basis vectors, which is especially interesting for joint dimension reduction and variable selection. To solve it, we propose to leverage variable splitting methods, with the crucial step then lying on the Stiefel manifold. The resolution of this subproblem, involving the orthonormality constraint, is achieved through a tailored majorization-minimization (MM) step. Numerical experiments on gene expression measurements illustrate the interest of the proposal.

**Index Terms**— Sparse PCA, Robust Subspace Recovery, Stiefel Manifold, ADMM, Majorization-Minimization.

## 1. INTRODUCTION

Principal components analysis (PCA) [1] is probably the most celebrated solution to the problem of linear subspace recovery. From a demeaned data matrix consisting of  $n$  samples of dimension  $p$ , denoted  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathbb{R}^{p \times n}$ , PCA consists in computing  $\tilde{\mathbf{X}} = \mathbf{U}_{\text{PCA}}^T \mathbf{X} \in \mathbb{R}^{k \times n}$  where  $\mathbf{U}_{\text{PCA}} \in \text{St}(p, k)$ <sup>1</sup> contains the  $k$  leftmost singular vectors of  $\mathbf{X}$ . This projection can serve for dimension reduction (from  $p$  to  $k < p$ ) and exploratory analysis. In comparison with non-linear dimension reduction methods (kernel methods [2], manifold embeddings [3] and autoencoders [4]), PCA has an advantage in the interpretability that comes from the recovered basis.

The standard PCA appears as the solution of various problem, such as orthogonal regression (least-squares subspace recovery), variance maximisation or maximum likelihood [5]. Nevertheless, this solution is prone to several issues, which motivated the derivation of alternative PCA algorithms with some desired properties:

*a) Robustness:* The standard PCA is sensitive to outliers, which can lead to irrelevant solutions when the sample set is

partially corrupted. Numerous approaches exist to overcome this issue, such as the use of robust estimators of the covariance matrix, or robust geometric costs [6]. These methods are broadly referred to as *robust subspace recovery* [7].

*b) Sparsity:* The standard PCA produces new variables that are linear combinations of all the original ones. Since these variables generally have a fundamental or physical meaning, such as assets in finance or genes in biology, a basis with only a few non-zero entries could facilitate the statistical interpretation and the variable selection. The problem of finding such vectors is referred to as *sparse PCA* and motivated numerous works (see e.g. [8–15] and references therein).

To enjoy the best of both worlds, [16] considered a robust sparse PCA formulation combining an  $M$ -estimation type fitting term [17, 18] and sparsity promoting penalties from [19]. In this paper, we propose a new algorithm suited to this approach that leverages variable splitting methods, see e.g. SOC [20] or the Manifold Alternating Direction Method of Multipliers (MADMM) [21]. Indeed, jointly handling the orthonormality constraint and sparsity promoting penalties is generally a hard task. The algorithms in [16] resort to smoothed penalties from [19] that allow to deal with the issue within the majorization-minimization framework. The proposed approach will allow for a direct use of non-smooth penalties. A notable interest is that it will newly permit the use of a mixed norm [22]. This type of penalty promotes structured sparsity patterns (e.g. *globally* sparse PCA [23, 24] or group Lasso [25]), which is useful in variable selection.

Though the proposed algorithm can be generalized to various robust costs functions (cf. [16]), this paper will focus on a Huber-type one, whose limit case yields the median subspace. The resulting algorithm will thus be referred to as median sparse PCA (MSPCA). Then, validation experiments on gene expression data will show that the proposed approach achieves a sparsity versus explained variance trade-off that is comparable to the state of the art, but without sacrificing the orthogonality of the basis vectors. It will also illustrate the interest of combining both robust subspace recovery fitting costs and sparse penalties.

In the following sections, let  $\mathbf{A}$  be a matrix with  $(i, j)^{th}$  entry  $[\mathbf{A}]_{i,j}$ ,  $i^{th}$  column  $\mathbf{a}_i$  and  $i^{th}$  row  $\mathbf{A}_{i,:}$ . Further on, we denote by  $\|\cdot\|_p$  the  $\ell_p$  norm, by  $\|\cdot\|_F$  the Frobenius one and the  $\ell_{2,1}$ -norm by  $\|\mathbf{A}\|_{2,1} \triangleq \sum_{i=1}^p \|\mathbf{A}_{i,:}\|_F$

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<sup>1</sup>Stiefel manifold, denoted as  $\text{St}(p, k) = \{\mathbf{U} \in \mathbb{R}^{p \times k} : \mathbf{U}^T \mathbf{U} = \mathbf{I}_k\}$

## 2. PROBLEM FORMULATION

We consider the following robust sparse PCA problem:

$$\begin{aligned} \min_{\mathbf{U}} \quad & \frac{1}{n} F_{q,\delta}(\mathbf{U}, \mathbf{X}) + \lambda \psi(\mathbf{U}) \\ \text{s.t.} \quad & \mathbf{U} \in \text{St}(p, k) \end{aligned} \quad (1)$$

where:

- $F_{q,\delta}$  is a robust Huber-type data-fitting cost [16, 17]:

$$F_{q,\delta}(\mathbf{U}, \mathbf{X}) = \sum_{i=1}^n \rho(\text{dist}(\mathbf{x}_i, \mathbf{U})) \quad (2)$$

with  $\text{dist}(\mathbf{x}_i, \mathbf{U}) = \|\mathbf{x}_i - \mathbf{U}\mathbf{U}^T \mathbf{x}_i\|_F$  and the function:

$$\rho(x) = \begin{cases} \frac{1}{2\delta} x^2 + (q\delta)^{q/(2-q)} - \frac{(q\delta)^{2/(2-q)}}{2\delta} & \text{if } x^{2-q} < q\delta \\ x^q & \text{if } x^{2-q} \geq q\delta \end{cases} \quad (3)$$

induces some robustness in the estimation process thanks to the use of a  $q$ -norm rather than a quadratic term for large errors. Typically,  $q = 1$  and a small  $\delta$  yield a tractable approximation of the median subspace. Otherwise, the classical least-squares subspace fitting is obtained for  $q = 2$ . The interest of  $F_{q,\delta}$  was evidenced in robust subspace recovery but not fully leveraged in (globally) sparse PCA with standard sparsity promoting penalties such as  $\ell_1$  and  $\ell_{2,1}$ -norms.

- $\psi(\cdot)$  is a sparsity promoting penalty and  $\lambda \in \mathbb{R}^+$  is a regularization parameter. For example, the  $\ell_1$ -norm promotes unstructured sparsity in the basis  $\mathbf{U}$ , while the  $\ell_{2,1}$ -norm promotes structured sparsity [25]. Its row-wise structure enforces the same sparsity pattern along all basis vectors, so as to reveal a subset of useful variables.

Even for the usual sparse PCA ( $q = 2$  and  $\ell_1$ -penalty), most works relax the orthogonality constraint on  $\mathbf{U}$  in (1). This approach tends to create correlated loading vectors at high regularization and thus degrade the explainability of the PCs. We will leverage MADMM to avoid such relaxation.

## 3. MADMM ALGORITHM

The problem (1) is difficult to handle due to the orthonormality constraint on  $\mathbf{U}$  and the non-smooth regularization penalty. We therefore consider a variable-splitting reformulation which will allow us to derive a tractable and efficient algorithm through MADMM [21], a special case of the renowned ADMM [26–28]. Indeed, we first formulate:

$$\begin{aligned} \min_{\mathbf{U}, \mathbf{V}} \quad & \frac{1}{n} F_{q,\delta}(\mathbf{U}, \mathbf{X}) + \lambda \psi(\mathbf{V}) \\ \text{s.t.} \quad & \mathbf{U} \in \text{St}(p, k), \mathbf{U} = \mathbf{V}. \end{aligned} \quad (4)$$

We keep the constraint  $\mathbf{U} \in \text{St}(p, k)$  while relaxing it on  $\mathbf{V}$  and conversely for the sparsity constraint. The constraint  $\mathbf{V} = \mathbf{U}$  implies that  $\mathbf{V}$  is eventually orthonormal and  $\mathbf{U}$  sparse, which allows for deriving practical updates of both variables. The augmented Lagrangian for (4) is:

$$L(\mathbf{U}, \mathbf{V}, \mathbf{\Gamma}) = \frac{1}{n} F_{q,\delta}(\mathbf{U}, \mathbf{X}) + \lambda \psi(\mathbf{V}) + \gamma \|\mathbf{U} - \mathbf{V}\|_F^2 + \langle \mathbf{\Gamma}, \mathbf{U} - \mathbf{V} \rangle \quad (5)$$

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### Algorithm 1 MADMM for MSPCA

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- 1: **Entry:**  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathbb{R}^{p \times n}$
  - 2: **Initialize**  $\mathbf{U} \in \mathbb{R}^{p \times k}$  (by PCA or another method)
  - 3: **Initialize**  $\mathbf{V} \in \mathbb{R}^{p \times k}$  randomly
  - 4: **Initialize**  $\mathbf{\Gamma} \in \mathbb{R}^{p \times k}$  by a matrix of zeros
  - 5: **repeat**
  - 6:     **Update**  $\mathbf{U}$  by following Algorithm 2
  - 7:     **Update**  $\mathbf{V}$  by following (15) or (16)
  - 8:     **Update**  $\mathbf{\Gamma}$  by :  $\mathbf{\Gamma} + 2\gamma(\mathbf{U} - \mathbf{V})$
  - 9: **until** convergence
  - 10: **Output:**  $\mathbf{U} \in \mathbb{R}^{p \times k}$
- 

with  $\gamma \in \mathbb{R}^+$ , and where  $\mathbf{\Gamma} \in \mathbb{R}^{p \times k}$  contains Lagrange multipliers associated with the constraint  $\mathbf{U} = \mathbf{V}$ . We then aim at alternatively minimizing this objective  $L$  for each variable, while keeping other fixed. Each step is detailed below and the full algorithm is summarized in Algorithm 1.

### 3.1. U-update

This step consists in fixing  $\mathbf{V}$  and  $\mathbf{\Gamma}$  and solving for a variable constrained to the Stiefel manifold:

$$\mathbf{U} = \underset{\mathbf{U} \in \text{St}(p, k)}{\text{argmin}} \quad L(\mathbf{U}, \mathbf{V}, \mathbf{\Gamma}), \quad (6)$$

Leaving out constant terms, we then consider:

$$\begin{aligned} \min_{\mathbf{U}} \quad & \frac{1}{n} F_{q,\delta}(\mathbf{U}, \mathbf{X}) + \gamma \|\mathbf{U} - \mathbf{V}\|_F^2 + \langle \mathbf{\Gamma}, \mathbf{U} - \mathbf{V} \rangle \\ \text{s.t.} \quad & \mathbf{U} \in \text{St}(p, k) \end{aligned} \quad (7)$$

The solution to this problem admits no closed-form solution. We therefore tailor a majorization-minimization algorithm in order to evaluate a local minimum of the objective function. The majorization step is applied thanks to the following proposition:

**Proposition 3.1.** *The objective function in (7) is majorized at point  $\mathbf{U}_t$  by the surrogate function:*

$$g(\mathbf{U}|\mathbf{U}_t) = -\text{Tr} \left( \mathbf{U}^T \left( \frac{q}{n} \tilde{\mathbf{X}} \tilde{\mathbf{X}}^T \mathbf{U}_t + 2\gamma \mathbf{V} - \mathbf{\Gamma} \right) \right) \quad (8)$$

with  $\tilde{\mathbf{X}} = [\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n]$  and  $\forall i = 1, \dots, n$ :

$$\tilde{\mathbf{x}}_i = \mathbf{x}_i / \max \left( \text{dist}^{(2-q)/2}(\mathbf{x}_i, \mathbf{U}_t), \sqrt{q\delta} \right). \quad (9)$$

Equality is achieved at  $\mathbf{U}_t$ .

*Proof.* First, we leverage the result of [17], stating that  $F_{q,\delta}$  can be majorized at point  $\mathbf{U}_t$  by the quadratic surrogate function

$$H_{q,\delta}(\mathbf{U}, \mathbf{X}|\mathbf{U}_t) = \frac{q}{2} \sum_{i=1}^n \text{dist}^2(\tilde{\mathbf{x}}_i, \mathbf{U}) + \text{const.} \quad (10)$$

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**Algorithm 2** U-Update
 

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- 1: **Entry:**  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathbb{R}^{p \times n}$
  - 2: **repeat**
  - 3:   **Form**  $\tilde{\mathbf{X}} = [\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n] \in \mathbb{R}^{p \times n}$
  - 4:   with  $\tilde{\mathbf{x}}_i = \mathbf{x}_i / \max \left( \text{dist}^{(2-q)/2}(\mathbf{x}_i, \mathbf{U}), \sqrt{q\delta} \right)$
  - 5:   **Compute**  $\mathbf{C} = \frac{q}{n} \tilde{\mathbf{X}} \tilde{\mathbf{X}}^T \mathbf{U} + 2\gamma \mathbf{V} - \mathbf{\Gamma}$
  - 6:   **Compute** the thin SVD:  $\mathbf{C} = \mathbf{U}_C \mathbf{\Sigma}_C \mathbf{V}_C^T$
  - 7:   **Update**  $\mathbf{U}$  by :  $\mathbf{U} = \mathbf{U}_C \mathbf{V}_C^T$
  - 8: **until** convergence
  - 9: **Output:**  $\mathbf{U} \in \mathbb{R}^{p \times k}$
- 

with  $\tilde{\mathbf{x}}_i$  defined in (9) (implicitly dependent on  $q$  and  $\delta$ ) and const. denoting a constant term w.r.t.  $\mathbf{U}$ . Now, remark that:

$$\begin{aligned} \sum_{i=1}^n \text{dist}^2(\tilde{\mathbf{x}}_i, \mathbf{U}) &= \sum_{i=1}^n \|\tilde{\mathbf{x}}_i - \mathbf{U} \mathbf{U}^T \tilde{\mathbf{x}}_i\|^2 \\ &= -\text{Tr}(\mathbf{U}^T \tilde{\mathbf{X}} \tilde{\mathbf{X}}^T \mathbf{U}) + \text{const.} \end{aligned} \quad (11)$$

Denote  $f_B(\mathbf{U}) = \text{Tr}(\mathbf{U}^T \tilde{\mathbf{X}} \tilde{\mathbf{X}}^T \mathbf{U})$ . The function  $-f_B(\mathbf{U})$  is quadratic concave, so it can be majorized at point  $\mathbf{U}_t$  by its first order Taylor expansion [29]:

$$\begin{aligned} -f_B(\mathbf{U}) &\leq -f_B(\mathbf{U}_t) - \text{Tr} \left( \left( \frac{\partial f_B(\mathbf{U}_t)}{\partial \mathbf{U}_t} \right)^T (\mathbf{U} - \mathbf{U}_t) \right) \\ &= -2 \text{Tr}(\mathbf{U}^T \tilde{\mathbf{X}} \tilde{\mathbf{X}}^T \mathbf{U}_t) + \text{const.} \end{aligned} \quad (12)$$

Adding the last two terms of (7), this linear majorizer yields the surrogate  $g$  as in (8).  $\square$

From the majorizer in Proposition 3.1, the minimization of the surrogate  $g$  is equivalent to:

$$\mathbf{U}_{t+1} = \underset{\mathbf{U} \in \text{St}(p, k)}{\text{argmax}} \text{Tr} \left( \mathbf{U}^T \left( \frac{q}{n} \tilde{\mathbf{X}} \tilde{\mathbf{X}}^T \mathbf{U}_t + 2\gamma \mathbf{V} - \mathbf{\Gamma} \right) \right) \quad (13)$$

which corresponds to an orthogonal Procrustes problem [30] whose solution can be computed as  $\mathbf{U}_{t+1} = \mathbf{U}_C \mathbf{V}_C^T$ , with the thin-SVD:  $\mathbf{C} \stackrel{\text{TSVD}}{=} \mathbf{U}_C \mathbf{\Sigma}_C \mathbf{V}_C^T$  and  $\mathbf{C} = \frac{q}{n} \tilde{\mathbf{X}} \tilde{\mathbf{X}}^T \mathbf{U}_t + 2\gamma \mathbf{V} - \mathbf{\Gamma}$ . The resulting algorithm to compute the  $\mathbf{U}$ -update is summarized in the box Algorithm 2.

### 3.2. V-update

Thanks to the variable splitting, this step consists simply in a proximal evaluation. Fixing  $\mathbf{U}$  and  $\mathbf{\Gamma}$ , we get:

$$\mathbf{V} = \underset{\mathbf{V}}{\text{argmin}} \gamma \left\| \tilde{\mathbf{U}} - \mathbf{V} \right\|_F^2 + \lambda \psi(\mathbf{V}), \quad (14)$$

with  $\tilde{\mathbf{U}} = \mathbf{U} + \frac{1}{2\gamma} \mathbf{\Gamma}$ . This gives the problem the form of a proximal [31] of the function  $\psi$ . If  $\psi$  is the  $\ell_1$ -norm, the solution is given by:

$$\mathbf{V} = S_{\lambda/2\gamma}(\tilde{\mathbf{U}}) \quad (15)$$

with the entry-wise soft-thresholding operator, defined (entry by entry) by:  $[S_{\lambda/2\gamma}(\tilde{\mathbf{U}})]_{ij} = \text{sgn}([\tilde{\mathbf{U}}]_{ij}) \left( |[\tilde{\mathbf{U}}]_{ij}| - \frac{\lambda}{2\gamma} \right)_+$  where  $(x)_+$  is the positive part function and  $\text{sgn}$  is the sign function. If  $\psi$  is the  $\ell_{2,1}$ -norm, the solution is given by:

$$\mathbf{V} = T_{\lambda/2\gamma}(\tilde{\mathbf{U}}) \quad (16)$$

with the row-wise thresholding operator, defined (row by row) by:  $[T_{\lambda/2\gamma}(\tilde{\mathbf{U}})]_i = \left( 1 - \frac{\lambda/2\gamma}{\|\tilde{\mathbf{U}}\|_1} \right)_+ [\tilde{\mathbf{U}}]_i$ .

For completeness, we mention the  $\mathbf{\Gamma}$ -update, a generic dual ascent step:  $\mathbf{\Gamma} \leftarrow \mathbf{\Gamma} + 2\gamma(\mathbf{U} - \mathbf{V})$

## 4. EXPERIMENTS

### 4.1. Simulation study for robustness

In the following, synthetic data will be drawn according to a Gaussian probabilistic model.

**Definition 4.1.** *Probabilistic PCA Model (PPCA) [5]*  
*Samples are drawn as a structured signal plus noise :*

$$\mathbf{x} = \mathbf{U}_0 \mathbf{s} + \mathbf{n} \quad (17)$$

with  $\mathbf{U}_0 \in \mathbb{R}^{p \times k}$ ,  $\mathbf{s} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \in \mathbb{R}^k$  and  $\mathbf{n} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}) \in \mathbb{R}^p$ . Then,  $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$  with  $\mathbf{\Sigma} = \mathbf{U}_0 \mathbf{U}_0^T + \sigma^2 \mathbf{I}$ .

Next, the outliers will be generated according to a Haystack-type model, which consists in a specific mixture of PPCA models, defined as follows.

**Definition 4.2.** *Haystack Model [32]*

*Samples  $\{\mathbf{x}_i\}_{i=1}^n$  are drawn as inliers and outliers as follows:*

$$\begin{aligned} \{\mathbf{x}_i\}_{i=1}^n &= \{\{\mathbf{x}_i^{in}\}_{i=1}^{n_{in}}, \{\mathbf{x}_i^{out}\}_{i=n_{in}+1}^n\} \\ \mathbf{x}^{in} &\sim \mathcal{N}(\mathbf{0}, \sigma_s^2 \mathbf{U}_0 \mathbf{U}_0^T + \mathbf{I}_p) \\ \mathbf{x}^{out} &\sim \mathcal{N}(\mathbf{0}, \sigma_o^2 \mathbf{U}_0^\perp (\mathbf{U}_0^\perp)^T + \mathbf{I}_p) \end{aligned} \quad (18)$$

where  $\mathbf{U}_0$  is the underlying signal subspace basis,  $\mathbf{U}_0^\perp \in \text{St}(p, p-k)$  is its orthonormal complement,  $\sigma_s^2$  and  $\sigma_o^2$  are respectively the signal and outlier to noise ratio while  $pc_o = (n - n_{in})/n$  is the fraction of outliers.

The sparse signal subspace basis  $\mathbf{U}_0$  is generated as:  $\mathbf{U}_0 = \begin{bmatrix} \mathbf{U}_d \\ \mathbf{0} \end{bmatrix}$ , Where  $\mathbf{U}_d \in \mathbb{R}^{d \times k}$ ,  $d \leq p$ , is an orthogonal basis and  $\mathbf{0} \in \mathbb{R}^{(p-d) \times k}$  is a matrix of zeros. For some resulting basis  $\mathbf{U}$ , the performance is evaluated in terms of average fraction of energy:

$$\text{AFE}(\mathbf{U}) = \mathbb{E} \left[ \text{Tr}(\mathbf{U}^T \mathbf{U}_0 \mathbf{U}_0^T \mathbf{U}) \right] / k \quad (19)$$

which assesses if the subspace spanned by  $\mathbf{U}_0$  is well recovered (on average) by the estimation process. The expectation is evaluated through 250 Monte-Carlo runs.

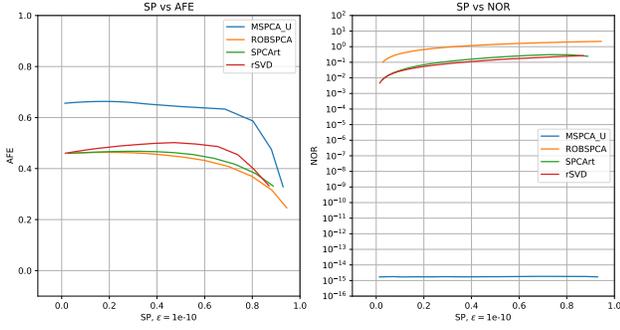


Fig. 1. AFE and NOR versus SP on synthetic data

This criterion will slightly favor the algorithms that relax the orthonormality constraint in PCA, so we also assess the non-orthogonality criterion  $\text{NOR}(\hat{\mathbf{U}}) = \|\hat{\mathbf{U}}^H \hat{\mathbf{U}} - \mathbf{I}\|_F^2$ . We measure these two criteria against the degree of sparsity of the basis:  $\text{SP}(\mathbf{U}) = 1 - \frac{\|\mathbf{U}\|_0}{p \times k}$ . The methods we compare against are rSVD [13], a vector-by-vector method with deflation from [33], SPCArt [14], a basis-wide method, and ROBSPCA [34].

Figure 1 shows the result of such a simulation with  $p = 100, k = 5, n = 100, d = 0.5p$  while  $\sigma_s = \sigma_o = \sqrt{10}$  and  $pc_o = 0.05$ . MSPCA is set with  $q = 1$  and  $\delta = 1$  (whose value does not dramatically impacting the results, as observed in [17]). It is evident that MSPCA, thanks to its robust cost, deals with outliers better than other methods from the leftmost plot: the AFE over all sparsity degrees is higher for MSPCA. From the rightmost plot we find out that MSPCA also respects more strictly the orthonormality constraint.

## 4.2. Study on a microarray gene dataset

Experiments are carried out on the Khan Gene Data [35], which consists of 2308 gene expression measurements from small round blue cell tumors of 63 patients across 4 classes (cancer types). We study the sparsity-performance trade-off of MSPCA using either  $\ell_1$ -norm or  $\ell_{2,1}$ -norm penalties. Since there is no ground truth for the ‘true’ underlying subspace, the AFE is computed as the fraction of recovered variance in  $\mathbf{X}$ .

Figure 2 displays the AFE and NOR versus the degree of row-sparsity (SProw). ROBSPCA and rSVD, not suited to structured sparsity, perform worse. We notice that MSPCA- $\ell_{2,1}$  achieves an AFE close to the one of SPCArt- $\ell_{2,1}$  (i.e., we modify SPCArt algorithm to use the  $\ell_{2,1}$ -norm penalty), while not relaxing the orthonormality constraints.

Finally, Figure 3 displays the first 3 principal components obtained with various algorithms: *i*) standard PCA; *ii*) MSPCA with no sparse penalty (equivalent to RSR in [17]); *iii*) MSPCA- $\ell_1$ ; *iv*) MSPCA- $\ell_{2,1}$ . All robust formulations use a Huber cost with  $q = 1$  and  $\delta = 1$ . The sparse penalties are set to obtain a similar sparsity (SP) level.

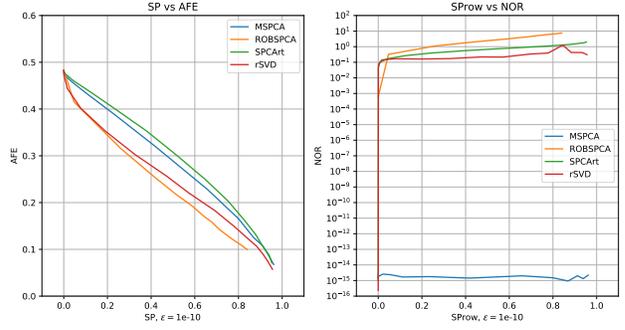


Fig. 2. AFE and NOR versus SProw of various sparse PCA algorithms on Khan Gene Data.

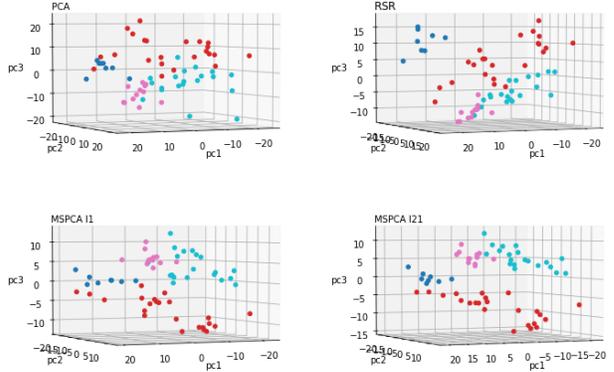


Fig. 3. Display of the 3 first principal components from PCA (top left), RSR (top right), MSPCA- $\ell_1$  (bottom left), MSPCA- $\ell_{2,1}$  (bottom right). Each color in the point cloud represents a different class (cancer type).

We notice the interest of the robust fitting criterion (2) compared to the standard least squares PCA formulation, as the obtained principal components separates the classes more clearly across the data points cloud (top row). We also observe that the sparse PCA approaches offer a projection where the classes appear more clearly separated (bottom-left). The proposed  $\ell_{2,1}$  penalty allows us to perform an interesting joint dimension reduction and variable selection, that improves the class separation (bottom-right) in an unsupervised manner.

## 5. CONCLUSION

This paper proposed a method to perform sparse PCA using a robust subspace recovery fitting and a non-smooth sparsity promoting penalty. Experiments on gene expression data showed both the interest of the approach in terms of explained variance versus sparsity trade-off, as well as for the visual representation of the principal components.

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