Learning Feature Sparse Principal Components

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Abstract

Sparse PCA has shown its effectiveness in high dimensional data analysis, while there is still a gap between the computational method and statistical theory. This paper presents algorithms to solve the row-sparsity constrained PCA, named Feature Sparse PCA (FSPCA), which performs feature selection and PCA simultaneously. Existing techniques to solve the FSPCA problem suffer two main drawbacks: (1) most approaches only solve the leading eigenvector and rely on the deflation technique to estimate the leading $m$ eigenspace, which has feature sparsity inconsistence, identifiability, and orthogonality issues; (2) some approaches are heuristics without convergence guarantee. In this paper, we present convergence guaranteed algorithms to directly estimate the leading $m$ eigenspace. In detail, we show for a low rank covariance matrix, the FSPCA problem can be solved globally (Algorithm 1). Then, we propose an algorithm (Algorithm 2) to solve the FSPCA for general covariance by iteratively building a carefully designed low rank proxy covariance. Theoretical analysis gives the convergence guarantee. Experimental results show the promising performance of the new algorithms compared with the state-of-the-art method on both synthetic and real-world datasets.

1 Introduction

Principal component analysis (PCA) (Pearson, 1901), is one of the most commonly used techniques for dimension reduction, which is a fundamental tool in a wide range of areas including machine learning, finance, genomics and many others. Vanilla PCA calculate the principal components of given samples by computing the leading eigenvectors of the sample covariance matrix.

In high dimension, with $d \gg n$, PCA has inconsistence issue in estimating the leading eigenvectors of population covariance matrix (Johnstone & Lu, 2009). Indeed, PCA will not be consistent if $d/n$ does not go to zero, that is the angle between the PCA estimate and the true leading principal components does not converge to zero. One way to address this issue is to assume the sparsity in the principal components. Prior work has been proposed in method design (Zou et al., 2006; Shen & Huang, 2008; d’Aspremont et al., 2007; Vu et al., 2013a; Yang & Xu, 2015; Kundu et al., 2017) and theoretical understanding (Vu et al., 2013b; Lei et al., 2015; Yang et al., 2016; Zhang & Han, 2018).

However, there remains a significant gap between the computational method and statistical theory of sparse PCA. No tractable algorithm is available to globally solve the spare PCA problem for general covariance matrix. This gap arises from the non-convex optimization formulation of sparse PCA. Several methods has been proposed to close this gap. d’Aspremont et al. (2007) propose a convex relaxation method named DSPCA for estimating the leading principal components. Vu et al. (2013b) extends DSPCA to estimate the $m$ leading eigenvectors.
A generalized power method is proposed in (Journée et al., 2010) to directly solve the non-convex problem. Generalized iterative threshold-type methods are also proposed to solve the sparse PCA problem (Ma et al., 2013; Yuan & Zhang, 2013). Solving the non-convex problem with Greedy search (dAspremont et al., 2008) or with a regression-type objective function (Jolliffe et al., 2003; Zou et al., 2006; Shen & Huang, 2008; Cai et al., 2013a) are also proposed.

Yet, there are some drawbacks in the existing methods. (1) Some non-convex optimization methods (Journée et al., 2010; dAspremont et al., 2008) consider cardinality regularized objective function rather than sparsity constraint, where the regularization hyper-parameter has to be carefully chosen to obtain specific sparsity. (2) Some methods (Yuan & Zhang, 2013; Ma et al., 2013; dAspremont et al., 2008; Yang & Xu, 2015) only estimates the leading eigenvector, and employs the deflation method (Mackey, 2009) to estimate the \( m \) leading eigenvectors, which leads to identifiability and orthogonality issues when the top \( m \) eigenvalues are not distinct. (3) Some approaches are heuristics without convergence guarantee.

In this paper, we provide two optimization strategies to directly estimate the row sparsity constrained \( m \) leading eigenvectors simultaneously, without deflation scheme. The first strategy (Algorithm 1) solves the feature sparse PCA problem globally when covariance matrix is low rank, while the second strategy (Algorithm 2) solves the feature sparse PCA for general covariance matrix iteratively with the convergence guaranteed.

**Contribution.** The main contributions of this paper is threefold.

- We show that, for a low rank covariance matrix, the FSPCA problem can be solved globally and provide an algorithm (Algorithm 1).
- For the general high rank covariance matrix, we report a convergence guaranteed iterative algorithm to solve it by building a carefully designed low rank proxy covariance for the FSPCA problem.
- Experimental results demonstrate the promising performance of the newly proposed algorithms compared with the state-of-the-art method on both synthetic and real-world datasets.

**Organization.** The rest of this paper is organized as follows. We review some closely related prior work in Section 2. The formal statement of FSPCA and some useful notions are put in Section 3. The newly proposed optimization strategies are in Section 4. Theoretical analysis of the new algorithms is in Section 5. We provide discussions on MM framework and the invertibility issue in Section 6. Experimental results on both synthetic and real-world datasets are provided in Section 7. Finally, conclude the paper in Section 8.

**Notation.** Throughout this paper, scalars, vectors and matrices are denoted by lowercase letters, boldface lowercase letters and boldface uppercase letters, respectively; for a matrix \( A \in \mathbb{R}^{n \times n} \), \( A^\top \) denotes the transpose of \( A \), \( \text{Trace}(A) = \sum_{i=1}^{n} a_{ii} \), \( \| A \|_F = \sqrt{\text{Trace}(A^\top A)} \); \( \mathbb{I}_n \in \mathbb{R}^n \) denotes vector with all ones; \( \| x \|_0 \) denotes the number of non-zero elements; \( \| A \|_{p,q} = \left( \sum_{i=1}^{n} \| a_{ii} \|_p^q \right)^{1/q} \); \( \mathbb{I}_{n \times n} \in \mathbb{R}^{n \times n} \) denotes the identity matrix; \( H_n = \mathbb{I}_{n \times n} - \frac{1}{n} \mathbb{I}_n \mathbb{I}_n^\top \) is the centralization matrix; \( I(1:k) \) is the first \( k \) elements in \( I \); \( A^\dagger \) denotes the Moore-Penrose inverse; \( \text{card}(I) \) is the cardinality of \( I \); \( \mathbb{1}\{\text{condition}\} \) is the indicator of the condition; RHS is the right-hand side. In this paper, we always assume the indices in \( I \) are sorted in ascending order.

## 2 Prior Arts

In this section, we review several prior work that is closely related to the problem concerned in this paper.

Most existing methods in the literature to solve the sparse PCA problem only estimate the leading eigenvector with sparsity constraint. Formally, the problem they consider solving is

\[
\max_{\| w \|_2 = 1, \| w \|_0 \leq k} w^\top A w.
\]
To estimate the $m$ leading eigenvectors, one has to build a new covariance matrix with the deflation technique (Mackey, 2009) and solve the leading eigenvector again. A main drawback of this scheme is that, for example, the indices of non-zero elements in the first eigenvector might not be that of the second eigenvector. The sparsity pattern is inconsistent among the $m$ leading eigenvectors. Moreover, the deflation has identifiability and orthogonality issues when the top $m$ eigenvalues are not distinct Wang et al. (2014).

In Vu et al. (2013b), they consider a different setting that the sparsity is forced consistent among rows, named row sparse PCA. In detail, they consider following problem

$$\max_{W \in \mathbb{R}^{m \times m}, \|W\|_{2,0} \leq k} \text{Trace} \left( W^\top A W \right),$$

which has nice statistical properties (Vu et al., 2013b). But there is a gap between the computational method and statistical theory. As pointed out in (Vu et al., 2013b), solving Row Sparse PCA problem is very difficult and has been proved to be NP-hard (Moghaddam et al., 2006). To close this gap, Wang et al. (2014) proposed an algorithm named Sparse Orthogonal iterAtion Pursuit (SOAP). SOAP solves exactly the same problem as that of this paper. But SOAP is not globally convergence guaranteed. We will see in Section 7.1, the objective function value curve of SOAP is not monotonic ascent.

Another line of research (Pang et al., 2018; Du et al., 2018; Cai et al., 2013b) consider solving sparse regression problem with the $\ell_{2,0}$ constraint. For example, the problem considered in (Pang et al., 2018) is

$$\min_{\|W\|_{2,0} \leq k} \|W^\top X + b\|_n^\top - Y\|_2,1$$

The main technical difference between the $\ell_{2,0}$ constrained sparse regression and row sparse PCA is the semi-orthogonal constraint on $W$. Without the semi-orthogonal constraint, the row sparse PCA problem is not bound from above. Thus, the problem considered in this paper is substantial difficult than that of $\ell_{2,0}$ constrained sparse regression.

### 3 Feature Sparse PCA

Assume centralized data, that is $XH_n = X$. The FSPCA problem can be rewritten as

$$\max_{W \in \mathbb{R}^{m \times m}, \|W\|_{2,0} \leq k} \text{Trace} \left( W^\top X X^\top W \right),$$

which is NP-hard even for $k = 1$ (Moghaddam et al., 2006). It is notable the FSPCA problem is equivalent to the row sparse PCA in Problem (1) with $q = 0$. In this paper, we propose algorithms to solve the following general problem

$$\max_{W \in \mathbb{R}^{m \times m}, \|W\|_{2,0} \leq k} \text{Trace} \left( W^\top A W \right),$$

where $m \leq k \leq d$ and matrix $A \in \mathbb{R}^{d \times d}$ is positive semi-definite.

**Remark 1.** It is notable the FSPCA problem can be viewed as performing feature selection and PCA simultaneously. The key point is the $\ell_{2,0}$ norm constraint forces the sparsity pattern consistence among different eigenvectors, while the vanilla sparse PCA model cannot keep this consistence.

We make following notion for ease of notations.

**Definition 1** (Row selection matrix map). We define $(d,k)$-row selection matrix map $S_{d,k}(I)$ to build row selection matrix $S \in \mathbb{R}^{d \times k}$ according to given indices $I$ such that $S_{d,k}(I) = S$. One can left multiply the row selection matrix $S$ to select specific $k$ rows from $d$ inputs. Specifically,

$$s_{ij} = \begin{cases} 
1 & \text{for } i = I(j) \\
0 & \text{for otherwise.}
\end{cases}$$

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Definition 2 (Set of the kth order principal submatrices). For $m \leq k \leq d$ and matrix $A \in \mathbb{R}^{d \times d}$, we define the set of the kth order principal submatrices of $A$ as

$$\mathcal{M}_k(A) = \{A_{I, I} : I \subseteq [d], \text{card}(I) = k \}.$$

4 Optimization Strategy

In this section, we provide new optimization strategies to solve the FSPCA model in Problem (2). We first consider the case when $\text{rank}(A) \leq m$, for which a non-iterative algorithm is provided to solve the problem globally. Then we consider the general case when $\text{rank}(A) > m$, for which an iterative algorithm is provided by approximating $A$ with a low rank proxy covariance $P_t$ and solving with the first case.

4.1 $\text{rank}(A) \leq m$

We start with an interesting observation. When we set $k = m$ in Problem (2) (do not require $\text{rank}(A) \leq m$), we are asking for the best $m$ features for projecting the original data into the best fit $m$ dimensional subspace. When features are independent, this setting seems reasonable. Specifically, the problem we are talking about is

$$\max_{W \in \mathbb{R}^{m \times m}, \|W\|_{2,0} \leq m} \text{Trace} \left( W^T A W \right).$$

Note that for each $W^T W = I_{m \times m}, \|W\|_{2,0} \leq m$, we can rewrite it as $W = SV$, where $V \in \mathbb{R}^{m \times m}$ satisfies $V^T V = I_{m \times m}$ and the row selection matrix $S \in \{0,1\}^{d \times m}$ satisfies $S^T 1_d = 1_m$. It is easy to verify, for given $A$, $\{S^T AS : S \in \{0,1\}^{d \times m}, S^T 1_d = 1_m \} = \mathcal{M}_m(A)$. Therefore, above problem is equivalent to

$$\max_{V \in \mathbb{R}^{m \times m}, \tilde{A} \in \mathcal{M}_m(A)} \text{Trace} \left( V^T \tilde{A} V \right).$$

(3)

Note that $V^T V = VV^T = I_{m \times m}$ since $V$ is square (which is not true when $k \neq m$). Combining with the fact $\text{Trace}(V^T \tilde{A} V) = \text{Trace}(\tilde{A} V V^T)$, Problem (3) can be rewritten as

$$\max_{\tilde{A} \in \mathcal{M}_m(A)} \text{Trace} \left( \tilde{A} \right),$$

which can be solved globally by sorting and selecting the $k$ largest diagonal elements of $\tilde{A}$.

If we consider above argument carefully, we will realize the key point is that by setting $k = m$, we are able to write $\sum_{i=1}^m \lambda_i(S^T AS)$ as $\text{Trace}(S^T AS)$. Equivalently, $\text{rank}(\tilde{A}) = \text{rank}(S^T AS) \leq m$.

Note that if $\text{rank}(A) \leq m$, then for all $k$ satisfying $m \leq k \leq d$, we have $\text{rank}(\tilde{A}) \leq m$ where $\tilde{A} \in \mathcal{M}_k(A)$. Thus, if $\text{rank}(A) \leq m$, we can use the same technique to solve the following problem even if $k \neq m$:

$$\max_{W \in \mathbb{R}^{m \times m}, \|W\|_{2,0} \leq k} \text{Trace} \left( W^T A W \right).$$

(4)

In detail, note that

$$\text{Prob. (4)} \iff \max_{\tilde{A} \in \mathcal{M}_k(A)} \sum_{i=1}^k \lambda_i(\tilde{A}) \iff \max_{\tilde{A} \in \mathcal{M}_k(A)} \text{Trace} \left( \tilde{A} \right),$$

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which can be easily solved globally by first sorting the diagonal elements of $A$ and selecting the $k$ largest elements then performing eigenvalue decomposition on the selected principal submatrix of $A$ to obtain $W$. The algorithm to solve Problem (4) is summarized in the following Algorithm 1.

**Algorithm 1** Solve Problem (4) with rank($A$) ≤ $m$

**Input:** feature sparsity $k$, the number of principal components $m$, covariance matrix $A \in \mathbb{R}^{d \times d}$ such that $m \leq k \leq d$ and rank($A$) ≤ $m$

1. Sort $\text{diag}(A)$ in descending order and put indices in $I$.
2. $\tilde{A} \leftarrow A_{I(1:k),I(1:k)}$.
3. $S \leftarrow S_{d,k}(I(1:k))$.
4. $V \leftarrow m$ leading eigenvectors of $\tilde{A}$.
5. $W \leftarrow SV$.

**Output:** $W \in \mathbb{R}^{d \times m}$ solves Problem (4).

4.2 rank($A$) > $m$

In this subsection, we consider the general case, that is, rank($A$) > $m$. When rank($A$) > $m$, the main difficulty prevents us from using the same technique shown in previous subsection is that $\sum_{i=1}^{m} \lambda_i(\tilde{A})$ cannot be written as $\text{Trace}(\tilde{A})$. Therefore, it cannot be solved by simply sorting and selecting. But we can try to build a proxy covariance, say $P$, of original $A$ such that rank($P$) ≤ $m$ and $P \succ 0$. Thus we can solve Problem (4) for $P$ to solve the original problem iteratively.

**Proxy Construction.** With careful design, given the estimate $W_t$ from the $t$th iterative step, we define matrix $P_t$

$$P_t = AW_t(W_t^\top AW_t)^\dagger W_t^\top A$$

as the proxy matrix of original $A$. Following claim verifies the condition for $P_t$ to be solvable with Algorithm 1.

**Claim 1.** For each $t \geq 1$, $W_t^\top W_t = I_{m \times m}$, it holds rank($P_t$) ≤ $m$, and $P_t \succ 0$.

**Proof.** The first part is from rank($P_t$) ≤ rank($W_t$) = $m$. Let $\Phi = AW_t(W_t^\top AW_t)^\dagger W_t^\top X$. Using the facts $A = XX^\top$ and $B^\dagger = B^\dagger BB^\dagger$, the second part is from

$$P_t = AW_t(W_t^\top AW_t)^\dagger W_t^\top XX^\top W_t(W_t^\top AW_t)^\dagger W_t^\top A = \Phi \Phi^\top \succ 0.$$

Indices Selection. With the proxy matrix $P_t$ in hand, a natural idea is to iteratively update $W$ by solving following problem with Algorithm 1:

$$\tilde{W}_{t+1} \leftarrow \arg \max_{W^\top W = I_{m \times m}, \|W\|_2 \leq k} \text{Trace}(W^\top P_t W). \quad (5)$$

Note that from Claim 1, above problem can be solved globally by simply sorting the diagonal elements of $P_t$ and selecting the rows and columns corresponding to the $k$ largest diagonal elements. Then the optimal $\tilde{W}_{t+1}$ can be obtained by performing eigenvalue decomposition on the $k$th order principal submatrix of $P_t$ and left multiplying it with a row selection matrix $S$. But we can further refine the $\tilde{W}_{t+1}$ by performing eigenvalue decomposition on original $A$ rather than on the proxy covariance $P_t$, which will accelerate the convergence.

**Eigenvectors Refinement.** Note that $\tilde{W}_{t+1}$ can be written as $\tilde{W}_{t+1} = S_{t+1} \tilde{V}_{t+1}$, which can be further refined by fixing the $S_{t+1}$ and updating $V_{t+1}$ with

$$V_{t+1} \leftarrow \arg \max_{V^\top V = I_{m \times m}} \text{Trace}(V^\top S_{t+1}^\top AS_{t+1} V). \quad (6)$$
And finally, the refined $\mathbf{W}_t$ can be computed by

$$\mathbf{W}_{t+1} \leftarrow \mathbf{S}_{t+1} \mathbf{V}_{t+1}.$$  

Compared with iterate with Problem (5), updating with the refinement makes larger progress thus it is more aggressive. The effect of the refinement stage will be demonstrated empirically in Section 7.2.

In summary, we collect the newly proposed procedure to solve FSPCA when $\text{rank}(\mathbf{A}) > m$ in Algorithm 2.

Algorithm 2 Solve Problem (2) with $\text{rank}(\mathbf{A}) > m$

**Input:** initial $\mathbf{W}_0$, feature sparsity $k$, the number of principal components $m$, covariance $\mathbf{A} \in \mathbb{R}^{d \times d}$ such that $m \leq k \leq d$ and $\text{rank}(\mathbf{A}) > k$

1: repeat
2: Proxy covariance construction:
   $$\mathbf{P}_t \leftarrow \mathbf{A} \mathbf{W}_t (\mathbf{W}_t^\top \mathbf{W}_t)^{\dagger} \mathbf{W}_t^\top \mathbf{A}.$$
3: Indices selection with Algorithm 1:
   $$\mathbf{W}_{t+1} \leftarrow \arg \max_{\mathbf{w}^\top \mathbf{w} = I_{m \times m}, \|\mathbf{w}\|_2 \leq k} \text{Trace} (\mathbf{W}_t \mathbf{P}_t \mathbf{W}_t).$$
4: Eigenvectors refinement:
   $$\mathbf{V}_{t+1} \leftarrow \arg \max_{\mathbf{v}^\top \mathbf{v} = I_{k \times k}} \text{Trace} (\mathbf{V}_t^\top \mathbf{S}_{t+1}^\top \mathbf{A} \mathbf{S}_{t+1} \mathbf{V}_t).$$
5: Update $\mathbf{W}_{t+1}$ with $\mathbf{W}_{t+1} \leftarrow \mathbf{S}_{t+1} \mathbf{V}_{t+1}$.
6: until converge

**Output:** $\mathbf{W} \in \mathbb{R}^{d \times m}$ solves Problem (4).

## 5 Theoretical Analysis

In this section, we provide convergence guarantee for the proposed iterative scheme to solve the general FSPCA problem. Since the concerned problem is NP-hard even when $k = 1$ (Moghaddam et al., 2006), we should not expect much in the deterministic setting. Our result shows that the iterative scheme in Algorithm 2 increases the objective function value in every iterative step. Combining with the fact that the objective function is bounded from above by finite $\text{Trace} (\mathbf{A})$, the convergence of Algorithm 2 can be guaranteed. Other than that, we provide computational complexity analysis on the Algorithm 1 and 2, which shows that the overall complexity of Algorithm 1 is $\mathcal{O}(\max\{d \log d, k^3\})$ the cost of every iterative step in Algorithm 2 is $\mathcal{O}(\max\{d \log d, k^3, dkm\})$ which is more efficient than SOAP (Wang et al., 2014).

### 5.1 Convergence Guarantee

In this section, we show the iterative scheme proposed in Algorithm 2 increases the objective function value in every iterative step, which directly indicates the convergence of the iterative scheme.

Before proving the ascent theorem, we first introduce some preliminary results.

**Lemma 1** (Horn et al. 1990, Theorem 1.3.22). For $\mathbf{A} \in \mathbb{R}^{n_1 \times n_2}, \mathbf{B} \in \mathbb{R}^{n_2 \times n_1}$ with $n_1 \leq n_2$, we have

$$\lambda_i(\mathbf{B} \mathbf{A}) = \begin{cases} 
\lambda_i(\mathbf{A} \mathbf{B}) & \text{for } 1 \leq i \leq n_1 \\
0 & \text{for } n_1 + 1 \leq i \leq n_2.
\end{cases}$$
Lemma 1 leads to an eigenvalue estimate that will be used in our main proof.

**Corollary 1.** Let \( \Gamma = X^\top W_t (W_t^\top XX^\top W_t)^\dagger W_t^\top X \). For the eigenvalues of \( \Gamma \), it holds

\[
\lambda_i(\Gamma) = \begin{cases} 
1 & \text{for } 1 \leq i \leq r \\
0 & \text{for } r + 1 \leq i \leq d,
\end{cases}
\]

where \( r = \text{rank}(X^\top W_t) \leq m \).

**Proof.** Let \( A = (W_t^\top XX^\top W_t)^\dagger W_t^\top X, B = X^\top W_t \). Thus, for each \( 1 \leq i \leq d \), \( \lambda_i(\Gamma) = \lambda_i(AB) \) and

\[
AB = (W_t^\top XX^\top W_t)^\dagger W_t^\top XX^\top W_t.
\]

Using Lemma 1, we have

\[
\lambda_i(\Gamma) = \begin{cases} 
\lambda_i(AB) & \text{for } 1 \leq i \leq m \\
0 & \text{for } m + 1 \leq i \leq n.
\end{cases}
\]

Note that \( \text{rank}(AB) = r \leq m \) and

\[
AB = \begin{bmatrix} I_{r \times r} & 0 \\ 0 & 0 \end{bmatrix},
\]

which completes the proof. \( \square \)

**Lemma 2** (Von Neumann 1937). Assume matrix \( X \in \mathbb{R}^{n \times n} \) and \( Y \in \mathbb{R}^{n \times n} \) are symmetric. Then,

\[
\text{Trace}(XY) \leq \sum_{i=1}^{n} \lambda_i(X)\lambda_i(Y).
\]

Now we are ready to prove the main result which shows the objective function values generated by Algorithm 2 are monotonic ascent.

**Theorem 1.** Let \( \tilde{W}_{t+1} \) be the optimum of Problem (5), which can be written as \( \tilde{W}_{t+1} = S_{t+1} \tilde{V}_{t+1} \). Let \( V_{t+1} \) be the optimum of Problem (6) and \( W_{t+1} = S_{t+1} V_{t+1} \). Assume \( A \) is positive semi-definite, say, \( A = XX^\top \). Then, it holds

\[
\text{Trace}(W_t^\top AW_t) \leq \text{Trace}(W_{t+1}^\top AW_{t+1}),
\]

that is, the iterative scheme proposed in Algorithm 2 makes objective function value monotonically increasing in every iterative step until convergence.

**Proof.** Note that

\[
\text{Trace}(W_t^\top AW_t) \overset{\oplus}{=} \text{Trace}(W_t^\top AW_t (W_t^\top AW_t)^\dagger W_t^\top AW_t) \overset{\ominus}{=} \text{Trace}(\tilde{W}_{t+1}^\top AW_t (W_t^\top AW_t)^\dagger W_t^\top A \tilde{W}_{t+1}) \overset{\ominus}{=} \text{Trace}(X^\top W_t (W_t^\top AW_t)^\dagger W_t^\top XX^\top \tilde{W}_{t+1} \tilde{W}_{t+1}^\top X)
\]

where \( \oplus \) uses fact \( A = AA^\dagger A \); \( \ominus \) uses \( \tilde{W}_{t+1} \) maximizing Problem (4); \( \ominus \) uses \( A \) is positive semi-definite (or \( A = XX^\top \)).

Let \( \Gamma \in \mathbb{R}^{d \times d}, \Omega \in \mathbb{R}^{d \times d} \) be

\[
\Gamma = X^\top W_t (W_t^\top AW_t)^\dagger W_t^\top X \quad \Omega = X^\top \tilde{W}_{t+1} \tilde{W}_{t+1}^\top X.
\]
Then, the RHS of $\mathcal{R}$ can be rewritten as

$$\text{RHS of } \mathcal{R} = \text{Trace}(\Gamma \Omega) \leq \sum_{i=1}^{d} \lambda_i(\Gamma) \lambda_i(\Omega) \leq \sum_{i=1}^{m} \lambda_i(\Omega),$$

where $\mathcal{R}$ uses Lemma 2; $\mathcal{G}$ uses Corollary 1 and fact for each $1 \leq i \leq m$, we have $\lambda_i(\Omega) \geq 0$.

Note that $\text{rank}(\Omega) \leq \text{rank}(\tilde{W}_t+1) = m$. Then we have $\sum_{i=1}^{m} \lambda_i(\Omega) = \text{Trace}(\Omega)$. Thus the RHS of $\mathcal{R}$ can be rewritten as

$$\text{RHS of } \mathcal{G} = \text{Trace}(\Omega) = \text{Trace}(\tilde{W}_t+1 \tilde{A} \tilde{W}_t+1),$$

which is exactly the updated objective function value of Problem (5). But we can go further by notice that $\tilde{W}_t+1 = S t+1 \tilde{V}_t+1$, $W_t+1 = S t+1 V_t+1$, and $V_t+1$ maximizes Problem (6). That gives

$$\text{Trace}(\tilde{W}_t+1 \tilde{A} \tilde{W}_t+1) = \text{Trace}(\tilde{V}_t+1^T S t+1 A S t+1 \tilde{V}_t+1) \leq \text{Trace}(W_t+1 \tilde{A} W_t+1),$$

which completes the proof.

**Remark 2.** Theorem 1 shows that the new proposed Algorithm 2 is ascent, that is $\{\text{Trace}(W_t^T A W_t)\}_{t=1}^{T}$ is an increasing sequence, which is important since most of the existing algorithm to solve Problem (2) cannot show their ascent. Combining with the fact that the objective function is bounded from above by finite $\text{Trace}(\tilde{A})$, the convergence of Algorithm 2 can be obtained.

### 5.2 Computational Complexity

In this subsection, we consider the computational complexity of Algorithm 1 and 2.

For Algorithm 1, it is easy to see the overall complexity is $O(\max\{d \log d, k^3\})$ since $O(d \log d)$ for indices selection, $O(k^2)$ for building $\tilde{A}$, $O(k^3)$ for eigenvalue decomposition of $\tilde{A}$, and $O(km)$ for building $W$.

For Algorithm 2, the overall computational complexity is $O(\max\{d \log d, k^3, dkm\})T$, where $T$ is the number of iterative steps used to coverage. In Section 7.1, we will see the number of iterative steps $T$ is usually less than 20 empirically. For proxy covariance construction and indices selection, we need $O(\max\{dn^2, d \log d\})$ for naively building $P_t$ and running Algorithm 1. But note that we only need the diagonal elements in $P_t$ for sorting and selecting. Thus, we only compute the diagonal elements of $P_t$ and sort it for the indices selection, that is $O(\max\{dkm, d \log d\})$. Then, performing eigenvectors refinement and updating $W_{t+1}$ costs $O(k^3)$. The computational complexity of SOAP proposed in (Wang et al., 2014) is $O(d^2m)$ for every iterative step. Ours computational complexity is strictly less than that of SOAP.

### 6 Discussion

In this section, we provide discussion to show that the newly proposed algorithm fits into the MM Framework and discuss the invertibility issue of $W_t^T A W_t$.

#### 6.1 MM Framework

Lots of classical algorithm can be framed into the MM framework, e.g., EM Algorithm (Dempster et al., 1977), Proximal Algorithms (Bertsekas & Tseng, 1994; Parikh et al., 2014), Concave-Convex Procedure (CCCP) (Yuille & Rangarajan, 2002; Lipp & Boyd, 2016). The algorithm solving vanilla sparse PCA proposed by Yuan & Zhang (2013) can also be framed into that framework. We refer the reader to (Sun et al., 2017) for further discussion.
It is notable that our algorithm can also be viewed as a special case of the general MM (Minorize-Maximization) algorithm with the auxiliary function defined by
\[ g(W; W_t) = \text{Trace}(W^\top AW_t(W_t^\top AW_t)^\dagger W_t^\top AW) \leq \text{Trace}(W^\top AW), \]
which satisfies \( g(W; W_t) = \text{Trace}(W_t^\top AW_t) \).

6.2 On the Invertibility \( W_t^\top AW_t \)

In the definition of the proxy matrix \( P_t \), there is a MoorePenrose inverse term \( (W_t^\top AW_t)^\dagger \). In this subsection we provide condition under which this matrix is invertible thus the MoorePenrose inverse can be replaced with matrix inverse. The reason why we care about the invertibility is that when \( W_t^\top AW_t \) is not invertible, it is rank deficient. Thus it might not be a good approximation to the high rank covariance \( A \). First of all, we need a result to bound the eigenvalues of principal submatrix.

**Lemma 3** (Horn et al. 1990, Theorem 4.3.28). Let \( A \in \mathbb{R}^{d \times d} \) be symmetric matrix that can be partitioned as
\[ A = \begin{bmatrix} B & C \\ C^\top & D \end{bmatrix}, \]
where \( B \in \mathbb{R}^{k \times k}, C \in \mathbb{R}^{k \times (d-k)}, D \in \mathbb{R}^{(d-k) \times (d-k)} \). Let the eigenvalues of \( A \) and \( B \) be sorted in descending order. Then, for each \( 1 \leq i \leq k \), we have \( \lambda_i(A) \geq \lambda_i(B) \geq \lambda_{d-k+i}(A) \).

**Claim 2.** If \( \text{rank}(A) \geq d - k + m \), then \( W_t^\top AW_t \) in Algorithm 2 is always invertible.

**Proof.** For ease of notation, we denote \( W_t \) by \( W \). Recall we can always extend the semi-orthonormal matrix \( W \) to an orthonormal matrix \( \overline{W} = [W \ W_\perp] \). We can write \( W^\top AW \) as a block since
\[ \overline{W}^\top \overline{W} = \begin{bmatrix} W^\top AW & W^\top AW_\perp \\ W_\perp^\top AW & W_\perp^\top AW_\perp \end{bmatrix}. \]
Note that for each \( 1 \leq i \leq d \), we have \( \lambda_i(\overline{W}^\top \overline{W}) = \lambda_i(A) \) since \( \overline{W} \) is orthonormal. Using Lemma 3, we have for each \( 1 \leq i \leq m \),
\[ \lambda_i(W_t^\top AW_t) \geq \lambda_{d-k+i}(W^\top AW) = \lambda_{d-k+i}(A). \]
Using \( \text{rank}(A) \geq d - k + m \), the proof completes. \( \square \)

**Remark 3.** Note that the condition shown in Claim 2 is easy to be satisfied. Indeed, we can solve Problem (2) with \( A_x = A + \varepsilon \cdot I_{d \times d} \). Thus, \( \text{rank}(A_x) = d \geq d - k + m \). Note that this small \( \varepsilon \) perturbation on \( A \) does not change the optimal \( W \) because \( \text{Trace}(W^\top A_x W) = \text{Trace}(W^\top AW) + \varepsilon m \), which is only a constant \( \varepsilon m \) added to the original objective function. Thus, the the optimal \( W \) remains unchanged.

7 Experimental Results

In this section, we provide experimental results to validate the effectiveness of the proposed method on both synthetic data and real-world datasets. In our experiments, we only compare our methods with the state-of-the-art method SOAP proposed by Wang et al. (2014). There are two reasons support our choice:

1. Most of the existing methods only solve the leading eigenvector and rely on the deflation technique to estimate the other eigenvectors, which causes the non-zero indices inconsistent among eigenvector. More importantly, they are not exactly solving the Problem (2).
2. In Wang et al. (2014), they have shown with experiments that SOAP outperform the other sparse PCA algorithm.

Thus, we only compare our algorithms with SOAP.
Table 1: Performance Comparison for SOAP, Algorithm 1, and Algorithm 2 on Toy Data Scheme 1–6. [mean(±std)]

| Scheme | Random Initialization | Convex Relaxation |
|--------|-----------------------|-------------------|
|        | Intersection Ratio | Relative Error | HF | Intersection Ratio | Relative Error | HF |
| 1      | SOAP 0.7263 (±0.0689) | 0.0258 (±0.0238) | 0.1800 | 0.7143 (±0.1201) | 0.0768 (±0.0441) | 0.0100 |
|        | Alg. 2 0.9654 (±0.0409) | 0.0000 (±0.0002) | 1.0000 | 0.9857 (±0.0431) | 0.0001 (±0.0005) | 0.9700 |
| 2      | SOAP 0.7736 (±0.1127) | 0.0298 (±0.0208) | 0.0700 | 0.7700 (±0.1053) | 0.0391 (±0.0253) | 0.0400 |
|        | Alg. 2 0.9720 (±0.0389) | 0.0000 (±0.0000) | 1.0000 | 0.9986 (±0.0143) | 0.0000 (±0.0000) | 1.0000 |
| 3      | SOAP 0.7586 (±0.1161) | 0.0402 (±0.0267) | 0.0500 | 0.7614 (±0.1219) | 0.0395 (±0.0292) | 0.0700 |
|        | Alg. 1 1.0000 (±0.0000) | 0.0000 (±0.0000) | 1.0000 | 1.0000 (±0.0000) | 0.0000 (±0.0000) | 1.0000 |
| 4      | SOAP 0.7668 (±0.0950) | 0.0099 (±0.0050) | 0.3000 | 0.7957 (±0.1425) | 0.0236 (±0.0292) | 0.1900 |
|        | Alg. 2 0.8334 (±0.0683) | 0.0001 (±0.0004) | 0.9700 | 0.9043 (±0.1016) | 0.0046 (±0.0070) | 0.5700 |
| 5      | SOAP 0.4366 (±0.0692) | 0.0546 (±0.0274) | 0.0100 | 0.4786 (±0.1511) | 0.1197 (±0.0465) | 0.0000 |
|        | Alg. 2 0.8260 (±0.0611) | 0.0004 (±0.0012) | 0.8900 | 0.8914 (±0.0864) | 0.0049 (±0.0058) | 0.3700 |
| 6      | SOAP 0.6032 (±0.0673) | 0.0123 (±0.0146) | 0.3600 | 0.8029 (±0.1312) | 0.0281 (±0.0263) | 0.1500 |
|        | Alg. 2 0.6136 (±0.0747) | 0.0105 (±0.0129) | 0.4100 | 0.8143 (±0.1243) | 0.0253 (±0.0245) | 0.1600 |

7.1 Synthetic Data

To show the effectiveness of the proposed method, we build a series of small-scale synthetic datasets, whose global optimum can be obtained by brute-force searching. Then we compare SOAP with our method with optimal indices and objective value in hand.

The performance measure we used are

- Intersection Ratio:
  \[
  \frac{\text{card} (\{\text{estimated indices}\} \cap \{\text{optimal indices}\})}{\text{sparsity } k}.
  \]

The reason we use Intersection Ratio is that FSPCA performs feature selection and PCA simultaneously. The Intersection Ratio can measure the Intersection between the indices return by algorithm and the optimal indices.

- Relative Error:
  \[
  \frac{\text{Trace} \left( \mathbf{W}^T \mathbf{A} \mathbf{W} \right) - \text{Trace} \left( \mathbf{W}^* \mathbf{A} \mathbf{W}^* \right)}{\text{Trace} \left( \mathbf{W}^* \mathbf{A} \mathbf{W}^* \right)}.
  \]

- Hit Frequency:
  \[
  \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}\{ \text{Relative Error} \leq 10^{-3} \},
  \]

where \( N \) is the number of repeated running. This measure shows the frequency of the algorithm approximately reach the global optimum.

For the synthetic data, we fix \( m = 3, k = 7, d = 20 \). We cannot afford large-scale setting since the brute-force searching space grows exponentially. We consider following six schemes:

1. \( \lambda(\mathbf{A}) = \{100, 100, 4, 1, \ldots, 1\} \).
2. \( \lambda(\mathbf{A}) = \{300, 180, 60, 1, \ldots, 1\} \).
3. \( \lambda(\mathbf{A}) = \{300, 180, 60, 0, \ldots, 0\} \).
4. \( \lambda(\mathbf{A}) = \{160, 80, 40, 20, 10, 5, 2, 1, \ldots, 1\} \).
5. \( \mathbf{X} \) is iid sampled from Unif[0, 1] and \( \mathbf{A} = \mathbf{X} \mathbf{X}^T \).
6. \( \mathbf{X} \) is iid sampled from \( \mathcal{N}(0, 1) \) and \( \mathbf{A} = \mathbf{X} \mathbf{X}^T \).

For Scheme 1 and 2, they are the synthetic data used in (Wang et al., 2014). But we trim them to fit our setting, that is \( m = 3, k = 7, d = 20 \). For Scheme 3, we validate the correctness that Algorithm 1 globally solves Problem (4). For Scheme 4, we use it to see the performance comparison when the \( \text{rank}(\mathbf{A}) \) is strictly larger than \( m \). For Scheme 5 and 6, we compare the
performance when data are generated from known distribution rather than using the eigenvalues fixed covariance.

To generate the synthetic data, we let $U$ be a realization from iid uniform distribution with elements in $[0, 1]$ and reorthonormalize it as the eigenvectors. Then the covariance matrix in Scheme 1–4 is built with $A = U\Lambda U^\top$. For Scheme 5 and 6, we first generate realization $X$ from uniform or Gaussian distribution. Then $A = XX^\top$.

![Figure 1: Convergence Curve of SOAP, Algorithm 2 with and without Refinement on ORL Face Dataset.](image)

![Figure 2: Performance Comparison for SOAP, Algorithm 2 on Real-world Datasets.](image)

Our results are shown in Table 1, where Random is for the random initialization and the Convex Relaxation is solving a convex relaxation problem proposed in Vu et al. (2013a) and use it as the initial $W$. Every scheme is independently run for 100 times and report the mean and standard error. For the Random setting, every realization $A$ is repeated run 20 times with different random initialization. Thus, in the random initialization setting, we run all algorithms $20 \times 100 = 2000$ times. The overall mean and variance are reported. From the Table 1, we get following insights:

- For almost all the cases, our algorithm outperforms SOAP.
- Our algorithm performs will even on the difficult cases (Scheme 4), where the rank of covariance are strictly greater then $m$.
- For well-conditioned cases, our algorithm reach global optimum with high frequency (Scheme 1 and 2), while SOAP does this.
- Algorithm 1 gives global optimal solution.

While our algorithm has deterministic global convergence guarantee, SOAP is only local convergence guaranteed with high probability. Moreover, for our algorithm, we make an eigenvectors refinement stage. It is of interest to see if this stage actually accelerates the convergence. In Figure 1, we run our algorithm with and without the refinement stage, and SOAP while recored the evolution of their objective function values. Following remarks would be interesting:
• Refinement accelerate the convergence procedure.
• Our algorithm is guaranteed ascent but SOAP is not.

On the start point in Figure 1, we note that these three algorithms starts from the same initialization (convex relaxation). But we did not plot the start point (step 0) in Figure 1 since the objective function value is too large (since it is a solution of relaxed problem) to make the figures readable.

7.2 Real-world Data

In this subsection, we report results on three real-world datasets. Since we cannot afford to brute-force search the optimal indices on a thousands dimensional covariance matrix, we use the Explained Variance, used in (Wang et al., 2014; Yang & Xu, 2015), to measure the performance. The Explained Variance is defined with

\[
\text{Explained Variance} = \frac{\text{Trace}(W^TXX^TW)}{\text{Trace}(XX^T)}.
\]

The results are reported in Figure 2. Following remarks would be interesting:
• Our algorithm consistently outperforms SOAP.
• Our algorithm gets large Explained Variance even with a small number of features.

8 Conclusion

In this paper, we present algorithms to directly estimate the row sparsity constrained leading \( m \) eigenvectors. We proposed Algorithm 1 to solve FSPCA for low rank covariance globally. For general high rank covariance, we propose Algorithm 2 to solve FSPCA by iteratively building a carefully designed low rank proxy covariance matrix. The convergence of Algorithm 2 is guaranteed with theoretical analysis. Experimental results show the promising performance of the new algorithms compared with the state-of-the-art method.

References

Bertsekas, D. P. and Tseng, P. Partial proximal minimization algorithms for convex pprogram- ming. *SIAM Journal on Optimization*, 4(3):551–572, 1994.

Cai, T. T., Ma, Z., Wu, Y., et al. Sparse pca: Optimal rates and adaptive estimation. *The Annals of Statistics*, 41(6):3074–3110, 2013a.

Cai, X., Nie, F., and Huang, H. Exact top-k feature selection via \( \ell_2,0 \)-norm constraint. In *Twenty-Third International Joint Conference on Artificial Intelligence*, 2013b.

d’Aspremont, A., El Ghaoui, L., Jordan, M. I., and Lanckriet, G. R. A direct formulation for sparse pca using semidefinite programming. *SIAM Review*, 49(3):434–448, 2007.

Dempster, A. P., Laird, N. M., and Rubin, D. B. Maximum likelihood from incomplete data via the em algorithm. *Journal of the Royal Statistical Society. Series B (methodological)*, pp. 1–38, 1977.

Du, X., Nie, F., Wang, W., Yang, Y., and Zhou, X. Exploiting combination effect for unsupervised feature selection by \( \ell_{2,0} \) norm. *IEEE Trans. Neural Netw. Learn. Syst.*, (99):1–14, 2018.

dAspremont, A., Bach, F., and Ghaoui, L. E. Optimal solutions for sparse principal component analysis. *Journal of Machine Learning Research*, 9(Jul):1269–1294, 2008.
Horn, R. A., Horn, R. A., and Johnson, C. R. *Matrix analysis*. Cambridge University Press, 1990.

Johnstone, I. M. and Lu, A. Y. On consistency and sparsity for principal components analysis in high dimensions. *Journal of the American Statistical Association*, 104(486):682–693, 2009.

Jolliffe, I. T., Trendafilov, N. T., and Uddin, M. A modified principal component technique based on the lasso. *Journal of Computational and Graphical Statistics*, 12(3):531–547, 2003.

Journée, M., Nesterov, Y., Richtárik, P., and Sepulchre, R. Generalized power method for sparse principal component analysis. *Journal of Machine Learning Research*, 11(Feb):517–553, 2010.

Kundu, A., Drineas, P., and Magdon-Ismail, M. Recovering pca and sparse pca via hybrid-(1,l2) sparse sampling of data elements. *The Journal of Machine Learning Research*, 18(1):2558–2591, 2017.

Lei, J., Vu, V. Q., et al. Sparsistency and agnostic inference in sparse pca. *The Annals of Statistics*, 43(1):299–322, 2015.

Lipp, T. and Boyd, S. Variations and extension of the convex–concave procedure. *Optimization and Engineering*, 17(2):263–287, 2016.

Ma, Z. et al. Sparse principal component analysis and iterative thresholding. *The Annals of Statistics*, 41(2):772–801, 2013.

Mackey, L. W. Deflation methods for sparse pca. In *Advances in Neural Information Processing Systems*, pp. 1017–1024, 2009.

Moghaddam, B., Weiss, Y., and Avidan, S. Spectral bounds for sparse pca: Exact and greedy algorithms. In *Advances in neural information processing systems*, pp. 915–922, 2006.

Pang, T., Nie, F., Han, J., and Li, X. Efficient feature selection via $l_{2,0}$-norm constrained sparse regression. *IEEE Transactions on Knowledge and Data Engineering*, 2018.

Parikh, N., Boyd, S., et al. Proximal algorithms. *Foundations and Trends® in Optimization*, 1(3):127–239, 2014.

Pearson, K. Liii. on lines and planes of closest fit to systems of points in space. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 2(11):559–572, 1901.

Shen, H. and Huang, J. Z. Sparse principal component analysis via regularized low rank matrix approximation. *Journal of Multivariate Analysis*, 99(6):1015–1034, 2008.

Sun, Y., Babu, P., and Palomar, D. P. Majorization-minimization algorithms in signal processing, communications, and machine learning. *IEEE Transactions on Signal Processing*, 65(3):794–816, 2017.

Von Neumann, J. *Some matrix-inequalities and metrization of matric space*. 1937.

Vu, V. Q., Cho, J., Lei, J., and Rohe, K. Fantope projection and selection: A near-optimal convex relaxation of sparse pca. In *Advances in Neural Information Processing Systems*, pp. 2670–2678, 2013a.

Vu, V. Q., Lei, J., et al. Minimax sparse principal subspace estimation in high dimensions. *The Annals of Statistics*, 41(6):2905–2947, 2013b.

Wang, Z., Lu, H., and Liu, H. Tighten after relax: Minimax-optimal sparse pca in polynomial time. In *Advances in neural information processing systems*, pp. 3383–3391, 2014.
Yang, D., Ma, Z., and Buja, A. Rate optimal denoising of simultaneously sparse and low rank matrices. *The Journal of Machine Learning Research*, 17(1):3163–3189, 2016.

Yang, W. and Xu, H. Streaming sparse principal component analysis. In *International Conference on Machine Learning*, pp. 494–503, 2015.

Yuan, X.-T. and Zhang, T. Truncated power method for sparse eigenvalue problems. *Journal of Machine Learning Research*, 14(Apr):899–925, 2013.

Yuille, A. L. and Rangarajan, A. The concave-convex procedure (cccp). In *Advances in Neural Information Processing Systems*, pp. 1033–1040, 2002.

Zhang, A. and Han, R. Optimal sparse singular value decomposition for high-dimensional high-order data. *Journal of the American Statistical Association*, pp. 1–40, 2018.

Zou, H., Hastie, T., and Tibshirani, R. Sparse principal component analysis. *Journal of Computational and Graphical Statistics*, 15(2):265–286, 2006.