Sparsistency and Agnostic Inference in Sparse PCA

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\textbf{Abstract}

The presence of a sparse “truth” has been a constant assumption in the theoretical analysis of sparse PCA and is often implicit in its methodological development. This naturally raises questions about the properties of sparse PCA methods and how they depend on the assumption of sparsity. Under what conditions can the relevant variables be selected consistently if the truth is assumed to be sparse? If the truth is not sparse, let alone unique, what can be said about the results of sparse PCA? We answer these questions by investigating the properties of the recently proposed Fantope projection and selection (FPS) method in the high dimensional setting. Our results provide general sufficient conditions for sparsistency of the FPS estimator. These conditions are weak and can hold in situations where other estimators are known to fail. On the other hand, without assuming sparsity or identifiability, we show that FPS provides a sparse, linear dimension-reducing transformation that is close to the best possible in terms of maximizing the predictive covariance.

\section{Introduction}

Sparse principal components analysis (PCA) is a relatively new and popular technique for simultaneous dimension reduction and variable selection in high dimensional data analysis [e.g., JTU03; ZHT06]. It combines the central idea of classic (or ordinary) PCA [Hot33; Pea01] with the notion of sparsity: it seeks linear transformations that reduce the dimension of the data, while depending on a small number of variables, but retain as much variation as possible. In the population setting, these linear transformations correspond to the projectors of the \(k\)-dimensional principal subspaces, spanned by the eigenvectors of the population covariance matrix. The appeal of sparsity is that it not only enhances interpretability, but it can yield consistent estimates when sparsity is truly present in the population, even in high dimensions [JL09].
The development of sparse PCA has taken a brisk pace over the past decade. Methodological developments include regularized estimators based on penalizing or constraining the variance maximization formulation of PCA [Jou+10; JTU03; WTH09], regression or low-rank approximation [SH08; ZHT06], convex relaxations [dAs+07; dBE08; Vu+13], two-stage procedures based on diagonal thresholding [JL09; PJ07], and algorithmic variations of iterative thresholding [Ma13; YZ13]. Theoretical developments including consistency, rates of convergence, minimax risk bounds for estimating eigenvectors and principal subspaces and detection have been established under various statistical models [AW09; BR13b; CMW13; JL09; Lou12; Ma13; VL12; VL13; Vu+13].

The presence of a sparse “truth” has been an explicit assumption in the theoretical analysis of sparse PCA and is often an implicit assumption in its methodological development. This naturally raises questions about the properties of sparse PCA methods and how they depend on the assumption of sparsity. Under what conditions can the relevant variables be selected consistently if the truth is assumed to be sparse? If the truth is not sparse, let alone unique, what can be said about the results of sparse PCA? The first question is essentially concerned with variable selection consistency, or sparsistency. The second question is a bit more slippery, because it essentially requires us to assume nothing beyond independence of the observations, i.e. to be agnostic. In this paper, we answer these questions by investigating the properties of the recently proposed Fantope projection and selection (FPS) method due to Vu et al. [Vu+13].

Sparsistency is the ability of an estimator to accurately select the correct subset of variables when applied to a random sample generated from a model where only a subset of variables is assumed to be relevant. Conditions under which sparsistency holds provide important insights about both the estimator and the model. They have been studied extensively in other high dimensional inference problems such as linear regression [FL01; MB06; Wai09; ZY06] and Gaussian graphical model selection [LF09; Rav+11; Rot+08]. In contrast, theoretical analyses of sparse PCA have mainly focused on consistency and rates of convergence in matrix norm, with relatively less progress on variable selection. An exception is Amini and Wainwright [AW09], who analyzed a semidefinite relaxation of sparse PCA [dAs+07]. They considered the $k = 1$ case and assumed a stringent spiked covariance model where the population covariance matrix is block diagonal and its leading eigenvector is assumed to have a small number of nonzero entries of constant magnitude. Their work is an important first step, but it leaves open whether or not their stringent conditions can be loosened and it also does not address the $k > 1$ case.

In the first part of this paper, we investigate the sparsistency of FPS under general conditions. FPS estimates the projector of the $k$-dimensional principal subspace spanned by the leading eigenvectors rather than individual eigenvectors. When $k = 1$, it reduces to the semidefinite relaxation proposed by d’Aspremont et al. [dAs+07]. Our main results, Theorems 1 and 2, give broad sufficient conditions under which FPS can exactly recover
the relevant variables. Roughly, the conditions are that (1) the relevant variables are not too correlated with the irrelevant variables (limited correlation), and (2) the leverages (diagonals of the projector) of the relevant variables are large enough. Interestingly, these conditions are analogous to so-called (1) “irrepresentability” and (2) “β-min” conditions for variable selection consistency of the Lasso [MB06; van11; ZY06]. To our knowledge, this is the first sparsistency result for principal subspaces. When \( k = 1 \), it generalizes the results of Amini and Wainwright [AW09] in several directions, the most important of which is that it relaxes their condition on a block-diagonal population covariance matrix.

The second part of this paper addresses the question of assumption-free interpretation of sparse PCA within a framework that we call agnostic inference. Our goal is to provide both analysis and interpretation of sparse PCA with essentially no assumptions beyond independence of observations. The terminology is borrowed from the learning theory literature where the chief concern is estimating a classifier or regression function without assumptions on the model [KSS94], however much of our perspective is influenced by earlier work on maximum likelihood under misspecification [Ber66; Hub67; Whi82], interpretations obtained by extending the maximum likelihood principle [Aka73], and the notion of persistence of high-dimensional linear predictors proposed by Greenshtein and Ritov [GR04]. Our point is that although FPS is derived under the assumption of sparsity, its results can still be interpreted even when sparsity does not hold. The main result (Theorem 4) is that without assuming sparsity or identifiability, FPS provides a sparse, linear dimension-reducing transformation that is close to the best possible in terms of maximizing the predictive covariance.

The remainder of the paper is organized as follows. Section 2 provides background on the sparse principal components/subspace problem, the FPS estimator, and the assumptions that we use in the paper. Section 3 describes our sparsistency results, while deferring the bulk of proofs to later in Section 5. Section 4 contains our results on agnostic inference and interpretation of FPS. Section 6 closes the paper with some discussion. Finally, we collect our notation below for our readers’ convenience.

**Notation**

For two matrices \( A, B \) with conformable dimensions, \( \langle A, B \rangle := \text{trace}(A^T B) \) denotes the trace inner product. For a vector \( v \in \mathbb{R}^k \) and \( q \in [0, \infty] \), \( \|v\|_q = (\sum_{i=1}^{k} |v_i|^q)^{1/q} \) is the \( \ell_q \) norm if \( 0 < q < \infty \); when \( q = 0 \), \( \|v\|_0 \) is the number of non-zero entries of \( v \); when \( q = \infty \), \( \|v\|_\infty = \max_{1 \leq i \leq k} |v_i| \). For a matrix \( A \in \mathbb{R}^{n \times m} \), and index sets \( J_1 \subseteq [n] \) and \( J_2 \subseteq [m] \), \( A_{J_1, J_2} \) denotes the \( |J_1| \times |J_2| \) submatrix of \( A \) consisting of rows in \( J_1 \) and columns in \( J_2 \), and \( A_{J_1} \) (\( A_{*, J_2} \)) denotes the submatrix consists of corresponding rows (columns). Given \( q_1, q_2 \in [0, \infty] \) and \( A \in \mathbb{R}^{n \times m} \), the matrix \( (q_1, q_2) \)-pseudonorm \( \|A\|_{q_1, q_2} \) is defined as \( (\|A_{1*}\|_{q_1}, \|A_{2*}\|_{q_1}, \ldots, \|A_{n*}\|_{q_1})_{q_2} \). As usual, the spectral norm of \( A \) is denoted \( \|A\| \) and
the Frobenius norm is $\|A\|_F := \langle A, A \rangle^{1/2}$. If $A$ is a symmetric matrix, $\lambda_j(A)$ denotes the $j$th largest eigenvalue of $A$. We will use $\Sigma$ to denote the $p \times p$ underlying true covariance matrix, whose ordered eigenvalues are $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$. For a square matrix $A$, $\text{diag}(A)$ denotes its diagonal vector. For a vector $v$, $\text{supp}(v)$ is the support of $v$ (the index set corresponding to non-zero entries).

## 2 Preliminaries

Let $\Sigma \in \mathbb{R}^{p \times p}$ be a symmetric matrix with spectral decomposition

$$\Sigma = \sum_{j=1}^{p} \lambda_j u_j u_j^T,$$

where $\lambda_1 \geq \cdots \geq \lambda_p$ are eigenvalues and $u_1, \ldots, u_p \in \mathbb{R}^p$ is an orthonormal basis of eigenvectors. The $k$-dimensional principal subspace of $\Sigma$ is the subspace spanned by $u_1, \ldots, u_k$. It is unique iff the spectral gap $\lambda_k - \lambda_{k+1} > 0$, and its projector (orthogonal projection matrix) is

$$\Pi = \sum_{j=1}^{k} u_j u_j^T = UU^T,$$

where $U$ is the orthonormal matrix with columns $u_1, \ldots, u_k$. Every subspace has a unique projector and so we will consider the principal subspace and $\Pi$ to be equivalent, and we will also assume that $k$ is known or fixed in advance.

### 2.1 Sparse principal subspaces

Estimation of the principal subspace requires at minimum that it be well-defined. When this is the case, we can consider $\Pi$ to be a mapping $x \mapsto \Pi x$ and so it makes sense to consider indices of the variables that $\Pi$ depends on. Since $\Pi$ is positive semidefinite, this is equivalent to the indices of the nonzero diagonal entries of $\Pi$, because row/column $i$ of $\Pi$ is nonzero if and only if $\Pi_{ii} \neq 0$.

**Definition 1 (SPS).** $\Sigma$ satisfies the **sparse principal subspace assumption with support set** $J$ if $\lambda_k(\Sigma) - \lambda_{k+1}(\Sigma) > 0$ and $\text{supp}(\text{diag}(\Pi)) = J$.

The SPS assumption is the minimal requirement for sparse principal subspace estimation, and the assumption will only be used in Section 3 in our investigation of sparsistency. The eigengap condition ensures that the principal subspace is identifiable, and the support set definition states that the principal subspace does not depend on variables outside of $J$. This corresponds to a notion of subspace sparsity introduced by Vu and Lei [VL13] called
\( \ell_0 \) row sparsity, and it can be shown that 
\( J = \bigcup_{j=1}^{k} \text{supp}(u_j) \) for any orthonormal basis 
\( \{u_1, \ldots, u_k\} \) of the principal subspace [VL13].

When SPS is assumed, the statistical inference problem considered in this paper is, in a
general setting, to estimate \( J \) from a noisy version \( S \) of \( \Sigma \). It may be helpful to think of
\( \Sigma \) as the covariance of a \( p \)-dimensional random vector and \( S = S_n \) as sample covariance
matrix of a random sample of size \( n \), but that is not strictly necessary for our theoretical
analysis. When there is a sample size \( n \), we will throughout the paper that it satisfies
\[
\log p \leq n
\]
The noisiness of \( S \) will be quantified by an entry-wise tail bound on
\( W := S - \Sigma \).

**Definition 2 (Sub-Gaussian concentration).** The input matrix \( S \) satisfies the sub-Gaussian
concentration assumption with scale factor \( \sigma \) if
\[
\max_{ij} \mathbb{P}( |W_{ij}| \geq t ) \leq 2 \exp \left( -4nt^2/\sigma^2 \right)
\]
for all \( 0 < t \leq \sigma \).

Sub-Gaussian concentration implies the following maximal inequality:
\[
\mathbb{P}( \|W\|_{\infty, \infty} \geq \sigma \sqrt{\log p/n} ) \leq 2p^{-2}.
\]
In other words, the maximum entry-wise error is bounded by \( \sigma \sqrt{\log p/n} \) with high proba-
bility. This fact will be the starting point of subsequent analysis of the sparsistency of the
FPS estimator introduced in Section 2.2.

**Remark.** The sub-Gaussian concentration condition is suitable for sample covariance ma-
trices if the random vector has sub-Gaussian tails (see Proposition 1 below). The theory
and method are general enough to cover all symmetric matrices \( \Sigma \) and an entry-wise ap-
proximation \( S \) such that
\[
\max_{ij} \mathbb{P}( |W_{ij}| \geq t ) \leq f(p, t),
\]
where the function \( f(p, t) \) may or may not involve the index \( n \). For example, in a random
graph model with \( p \) nodes where edges appear independently with probability \( c_{jk} \) for all
\( 1 \leq j < k \leq p \). Let \( A \) be the random adjacency matrix, then the pair \( S = AA^T/(p-1) \) and
\( \Sigma = \mathbb{E}(S) \) satisfy the sub-Gaussian concentration assumption with \( n = 1 \). More generally,
our results do not even have to assume that \( \Sigma \) or \( S \) are positive semidefinite.

The following result gives a sufficient condition for (1) to hold for the sample covariance ma-
trix of an i.i.d. sample. The proof is a straightforward application of Bernstein’s inequality
[see vW96, Chapter 2.2] and omitted.
Proposition 1 (Concentration of sample covariance). Let $X, X_1, X_2, \ldots, X_n \in \mathbb{R}^p$ be i.i.d. random vectors with $\text{Var}(X) = \Sigma \succeq 0$ and let $S$ be the sample covariance matrix:

$$S = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})(X_i - \bar{X})^T,$$

where $\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$. If there exists a constant $C > 0$ such that

$$\sup_{\|v\|_2 = 1} \mathbb{P} \left( |v^T (X - \mathbb{E}X)| \geq t \right) \leq \exp \left[ -Ct^2/(v^T \Sigma v) \right],$$

then there is an absolute constant $c > 0$ such that $S$ satisfies (1) with $\sigma = c \lambda_1$.

2.2 Fantope projection and selection

Vu et al. [Vu+13] recently proposed an estimator for $\Pi$, called Fantope projection and selection (FPS), defined as a solution $\hat{H}$ to the following semidefinite program.

$$\hat{H} := \arg\max \left\{ \langle S, H \rangle - \rho \|H\|_{1,1} \right\} \text{ subject to } H \in F^k,$$

(2)

where $F^k := \{ H : 0 \preceq H \preceq I \text{ and } \text{trace}(H) = k \}$ is the trace-$k$ Fantope, and $\rho$ is a tuning parameter. Vu et al. [Vu+13] showed that FPS can be efficiently computed by alternating direction method of multipliers [ADMM, e.g., Boy+10]. When $\rho = 0$, a solution is given by the projector of the $k$-dimensional principal subspace of $S$ (see Lemma 1 below). The $\ell_1$ penalty term encourages the solution to be sparse, and the decomposability of this penalty term gives the solution $\hat{H}$ good statistical properties as an estimator for $\Pi$. In the next section, we will show that, if $\Sigma$ and $S$ satisfy both the SPS and sub-Gaussian concentration assumptions, then under mild conditions, $\text{supp}[\text{diag}(\hat{H})] = J$ with high probability for appropriate choices of $\rho$.

In general, the solution to (2) and hence the FPS estimator may not be unique. However, we will show that it is unique with high probability when the SPS and sub-Gaussian concentration assumptions hold. The argument utilizes the following elastic net version of FPS.

$$\min \left\{ -\langle S, H \rangle + \rho \|H\|_{1,1} + \frac{\tau}{2} \|H\|_F^2 \right\} \text{ subject to } H \in F^k.$$  

(3)

Since the objective is a strongly convex function, the solution of (3) is unique. A very interesting and important fact is that when $\rho$ and $\tau$ are small enough, if a solution of (2) is sparse then it must be the unique solution of (3). This observation will be proved in Section 5 and play a key role in establishing the uniqueness of solution for the original FPS problem.
We conclude this section by introducing some basic properties of the Fantope, which will be used repeatedly in the proof of main results. Further properties and discussion of the Fantope will be given in Section 4. Denote the Euclidean projection of a $p \times p$ symmetric matrix $A$ onto $\mathcal{F}^k$ by $P_{\mathcal{F}^k}(A) := \arg \min_{Z \in \mathcal{F}^k} \|A - Z\|_F^2$.

**Lemma 1** (Basic Properties of Fantope Projection). Let $A$ be a symmetric matrix with eigenvalues $\gamma_1 \geq \cdots \geq \gamma_p$ and orthonormal eigenvectors $v_1, \ldots, v_p$.

1. $\max_{H \in \mathcal{F}^k} \langle A, H \rangle = \gamma_1 + \cdots + \gamma_k$ and the maximum is achieved by the projector of a $k$-dimensional principal subspace of $A$. Moreover, the maximizer is unique if and only if $\gamma_k > \gamma_{k+1}$.
2. $P_{\mathcal{F}^k}(A) = \sum_j \gamma^+_j(\theta)v_jv_j^T$, where $\gamma^+_j(\theta) = \min(\max(\gamma_j - \theta, 0), 1)$ and $\theta$ satisfies the equation $\sum_j \gamma^+_j(\theta) = k$.
3. If $0 < \tau \leq \gamma_k - \gamma_{k+1}$, then

$$\arg \max_{H \in \mathcal{F}^k} \langle A, H \rangle = \arg \max_{H \in \mathcal{F}^k} \langle A, H \rangle - \frac{\tau}{2}\|H\|_F^2 = P_{\mathcal{F}^k}(\tau^{-1}A) = \sum_{j=1}^k v_jv_j^T,$$
uniquely.

**Proof.** (1) See Overton and Womersley [OW92]. (2) is Lemma 4.1 of Vu et al. [Vu+13]. (3) We have

$$\langle A, H \rangle - \frac{\tau}{2}\|H\|_F^2 = -\frac{\tau}{2}\|H - \tau^{-1}A\|_F^2 + \frac{1}{2\tau}\|A\|_F^2.$$ 

This is maximized over $H \in \mathcal{F}^k$ by $H = P_{\mathcal{F}^k}(\tau^{-1}A)$. Note that by assumption $\gamma_k/\tau \geq 1$ and $\gamma_{k+1} < \gamma_k$. Then the claim follows by applying (1) and (2).

3 **Sparsistency**

In this section we prove variable selection consistency of the FPS estimator. Throughout this section, we assume that $\Sigma$ satisfies SPS condition with dimension $k$ and active variable set $J = \{1, 2, \ldots, s\}$ for some $s \ll p$, and that $S$ satisfies the sub-Gaussian concentration condition with some $\sigma > 0$. The sample covariance matrix is covered as a special case in view of Proposition 1.

Intuitively, variable selection would be easier if the relevant variables (those in $J$) and noise variables (those in $J^c$) are not too correlated. In the context of sparse linear regression, such an intuition leads to the famous Irrepresentable Condition [Wai09; ZY06]. In sparse...
subspace estimation, we have the analogous Limited Correlation Condition (LCC). In order to state the condition concisely, we use the following block representation of $\Sigma$.

$$
\Sigma = \begin{pmatrix}
\Sigma_{JJ} & \Sigma_{JcJ} \\
\Sigma_{cJ} & \Sigma_{cJc}
\end{pmatrix}.
$$

Similar block representations can be defined for $S$ and $W = S - \Sigma$.

Our main technical condition, the limited correlation condition (LCC) is given below.

**Definition 3 (LCC).** A symmetric matrix $\Sigma$ satisfies the limited correlation condition with constant $\alpha \in (0, 1]$ ($\alpha$-LCC) if

$$
\frac{8s}{\lambda_k(\Sigma) - \lambda_{k+1}(\Sigma)}\|\Sigma_{cJ}\|_{2,\infty} \leq 1 - \alpha.
$$

The LCC contains the condition assumed by Amini and Wainwright [AW09] as a special case, where $\Sigma_{JcJ} = 0$ and hence LCC holds with $\alpha = 1$. Another popular model for sparse PCA is the spiked covariance model, where $\lambda_k(\Sigma_{JJ}) \geq c$, $\Sigma_{JcJc} = cI_{p-s}$, and $\Sigma_{cJ} = 0$. An important difference between LCC and the assumptions in previous works is that previous assumptions, for example, the spiked covariance model, usually imply that the relevant variables can be selected with good accuracy by thresholding the diagonal entries, while LCC contains situations where such diagonal thresholding intuition does not work. Here we illustrate this difference by a toy example with $p = 3$, $k = 1$, $J = \{1, 2\}$.

$$
\Sigma = \begin{pmatrix}
0.9 & 0.8 & t \\
0.8 & 0.9 & -t \\
t & -t & 1
\end{pmatrix}.
$$

This $\Sigma$ satisfies LCC with $\alpha = 0.3$ for any $|t| \leq 0.02$, but picking large diagonal entries of $\Sigma$ does not select the relevant variables.

To our knowledge, the LCC is the first sufficient condition for consistent sparse PCA variable selection without assuming $\Sigma$ being block-diagonal and is also the first sufficient condition for sparse subspace variable selection consistency.

### 3.1 Probabilistic guarantee for support recovery (main result)

When the input matrix $S$ is random and satisfies the sub-Gaussian concentration, we have the following probabilistic result on variable selection consistency of FPS.

**Theorem 1.** Assume that $\Sigma$ satisfies SPS and $\alpha$-LCC, and that $S$ satisfies the entry-wise sub-Gaussian concentration with scaling factor $\sigma$. If

$$
s\sqrt{\frac{\log p}{n}} < \frac{\alpha(\lambda_k - \lambda_{k+1})^2}{4\sigma(8\lambda_1 + \lambda_k - \lambda_{k+1})},
$$

8
and
\[ \rho = \sigma \frac{\log p}{\alpha n}, \]
then with probability at least \(1 - 2p^{-2}\) the optimizer \(\hat{H}\) of (2) is unique and satisfies
\[ \text{supp}(\text{diag}(\hat{H})) \subseteq J. \]
Furthermore, assuming in addition that one of the following holds
1. \[ s \sqrt{\frac{\log p}{n}} < \alpha \frac{(\lambda_k - \lambda_{k+1})}{4\sigma} \min_{j \in J} \sqrt{\Sigma_{jj}}, \] \[ \text{(5)} \]
2. \[ \text{rank}(\text{sign}(\Sigma_{JJ})) = 1, \quad \text{and} \quad \sqrt{\frac{\log p}{n}} < \frac{\alpha}{2\sigma} \min_{(i,j) \in J^2} \Sigma_{ij}, \] \[ \text{(6)} \]
then the FPS solution satisfies
\[ \text{supp}(\text{diag}(\hat{H})) = J. \]

The proof of Theorem 1 is given in Section 3.4, after introducing the deterministic sufficient conditions for sparsistency. The strategy is to show that, with high probability, the chosen \(\rho\) satisfies the deterministic sufficient conditions (Theorem 2 and lemmas 2 and 3) under which we have \(\text{supp}(\text{diag}(\hat{Z})) = J\).

Remark. When the eigenvalues of \(\Sigma\) are constants and do not change with \((n, p, s)\), Theorem 1 recovers a rate developed by Amini and Wainwright [AW09] as a special case where Theorem 1 implies that a sufficient condition for consistent variable selection (with suitable choice of \(\rho\)) is \(s \sqrt{\log p/n} \leq c\) for a constant \(c\) (according to (4) and (6)). Amini and Wainwright [AW09] also obtain a sharper sufficient condition \(s \log p/n \leq c'\), by assuming that the solution is rank 1. However [KNV13] show that, with high probability, the solution is not rank 1 unless \(s \sqrt{1/n}\) is bounded by a constant.

Next we establish the key intermediate result in proving Theorem 1: sparsistency for the FPS estimator with deterministic input. First we will establish that, under LCC, the FPS solution has no false positive: \(\text{supp}(\text{diag}(\hat{H})) \subseteq J\). Second, full sparsistency is established under additional condition of minimum signal strength.
3.2 False positive control under LCC

We first present a deterministic result that specifies the appropriate choices of \( \rho \) so that there is no false positive among the variables picked by FPS.

**Theorem 2** (Deterministic false positive control). Assume \( \Sigma \) satisfies the SPS condition. If

\[
\rho^{-1}\|S - \Sigma\|_{\infty,\infty} + \frac{8s}{\lambda_k - \lambda_{k+1}}\|\Sigma_{J^c}J\|_{2,\infty} \leq 1, \tag{7}
\]

\[
0 < \lambda_d - \lambda_{d+1} - 4\rho s \left(1 + \frac{8\lambda_1}{\lambda_k - \lambda_{k+1}}\right). \tag{8}
\]

then the solution of FPS problem (2) is unique and satisfies \( \text{supp}(\text{diag}(\hat{H})) \subseteq J \).

(7) reveals the motivation for LCC. When \( \alpha \)-LCC holds, one can choose \( \rho = \|S - \Sigma\|_{\infty,\infty}/\alpha \) so that (7) holds. On the other hand, (8) puts some upper bound constraint on \( \rho \). When \( S \) is random and satisfies the sub-Gaussian concentration condition, \( \|S - \Sigma\|_{\infty,\infty} \) depends on \( (n, p, \sigma) \). Then (7) and (8) jointly put a constraint on \( (s, p, n, \sigma, \lambda_1, \lambda_k, \lambda_{k+1}) \) so that there exists a \( \rho \) satisfying both conditions.

**Sketch of proof of Theorem 2.** The proof of Theorem 2, as given in Section 5.1, consists of two main parts. The first part (Section 5.1.1) is to show that there exists a solution of the FPS problem (2) supported on \( J \), using on the primal dual witness (PDW) argument [AW09; Rav+11; Wai09]. The PDW argument first constructs a sparse solution \( \hat{H} \) supported on \( J \) by solving the FPS problem (2) under additional sparsity constraint \( \text{supp}(\text{diag}(H)) \subseteq J \). Then it is shown that when \( \rho \) is large enough, with high probability one can find a dual variable \( \hat{Z} \) such that the primal-dual pair \((\hat{H}, \hat{Z})\) satisfies the KKT condition and hence is optimal for the original problem. When the solution is unique, this ensures that the optimizer is supported on \( J \). The challenge here is to establish KKT condition when \( \Sigma \) is not block diagonal, which requires a careful and delicate subspace perturbation analysis in comparing the FPS solution and the population projector (Lemmas 5 and 6).

The second part is to show that, under the conditions assumed in the theorem, the sparse solution constructed in the primal dual witness argument is indeed of rank \( k \) and also unique. Our proof of uniqueness is novel and makes use of the elastic net version of FPS (3). A key fact used in the proof is that, for small enough values of \( \tau \), the two problems have the same solution and the uniqueness of FPS solution follows essentially from that of the elastic net version. The details are given in Section 5.1.2.
3.3 False negative control

Having established false positive control in Theorem 2, full sparsistency will be established if we can show that the number of false negatives is also zero. In sparsity pattern recovery, the number of false negatives is typically controlled by assuming a lower bound on the magnitude of signals carried by relevant variables. In the context of principal subspace estimation, we give two different sufficient conditions that guarantee zero false negatives for the FPS output.

3.3.1 False negative control under minimum row norm condition.

Our first condition on signal strength is motivated by the following result by Vu et al. [Vu+13].

**Theorem 3 ([Vu+13]).** Assuming $\Sigma$ satisfies SPS, and that $\rho \geq \|W\|_{\infty, \infty}$, then the FPS solution $\hat{H}$ satisfies

$$\|\hat{H} - \Pi\|_F \leq \frac{4\rho_s}{\lambda_k - \lambda_{k+1}}.$$ 

Since $\Pi_{jj} = \|U_s\|_2^2$, Theorem 3 immediately suggests the following lemma.

**Lemma 2 (Sparsistency under row norm condition).** Under the conditions of Theorem 2, if

$$\min_{j \in J} \sqrt{\Pi_{jj}} > \frac{4\rho_s}{\lambda_k - \lambda_{k+1}},$$

then the FPS solution satisfies

$$\text{supp(diag(\hat{H}))} = J.$$ 

3.3.2 False negative control under entry-wise condition

Another sufficient condition for controlling false negative in FPS is motivated by an assumption used by Amini and Wainwright [AW09] for the $k = 1$ case where the leading eigenvector is assumed to be $v_1 = (1_s/\sqrt{s}, 0)$ (where $1_s$ is the $s \times 1$ vector of ones, and the signs of non-zero entries can actually be arbitrary) and $\Sigma_{JJ} = \theta v_1 v_1^T + I_s$. Let $\text{sign}(\Sigma_{JJ})$ be the $s \times s$ matrix of entry-wise signs of $\Sigma_{JJ}$. We generalize this condition as follows.

**Lemma 3.** Under the conditions of Theorem 2, if

$$\text{rank}((\Sigma_{JJ}))) = 1 \text{ and } \min_{(i,j) \in J^2} |\Sigma_{ij}| > 2\rho,$$

then the FPS solution satisfies $\text{supp(diag(\hat{H}))} = J.$
Proof of Lemma 3. It suffices to prove that the number of false negatives is zero. According to Theorem 2, we know that \( \hat{H} \) is supported on \( J \), and \( \hat{H}_{JJ} \) corresponds to the projector of the \( k \)-dimensional principal subspace of \( \hat{\Sigma}_{JJ} := S_{JJ} - \rho \hat{Z}_{JJ} \) where \( \hat{Z} \) is the optimal dual variable.

Then it is sufficient to show that the leading eigenvector of \( \hat{\Sigma}_{JJ} \) does not have zero entries. Note that \( \|\hat{\Sigma}_{JJ} - \Sigma_{JJ}\|_{\infty, \infty} \leq 2\rho \) and the second part of assumption (10) implies that \( \operatorname{sign}(\hat{\Sigma}_{JJ}) = \operatorname{sign}(\Sigma_{JJ}) \).

By the first part of assumption (10), we have \( \operatorname{sign}(\hat{\Sigma}_{JJ}) = \operatorname{sign}(\Sigma_{JJ}) = bb^T \), where \( b \in \{-1, 1\}^s \). Let \( B \) be the \( s \times s \) diagonal matrix such that \( \operatorname{diag}(B) = b \). The matrix \( B \hat{\Sigma}_{JJ} B \) has all positive entries and hence by the Perron-Frobenius Theorem, it has a unique leading eigenvector \( v_1 \) whose entries are all positive. As a result, the leading eigenvector of \( \hat{\Sigma}_{JJ} \) is \( Bv_1 \), which does not have zero entries.

\[ \]  

3.4 Proof of Theorem 1

Proof of Theorem 1. Using the sub-Gaussian concentration condition, with probability at least \( 1 - 2p^{-2} \) we have \( \rho^{-1}\|S - \Sigma\|_{\infty, \infty} \leq \alpha \). This together with the \( \alpha \)-LCC of \( \Sigma \) establishes (7). On the other hand, (4) ensures that (8) holds. Then the first part is proved using Theorem 2.

For the second part, (5) implies (9). Then the claim follows from Lemma 2. If (6) holds, then the claim follows with the same choice of \( \rho \) by applying Lemma 3.

\[ \]

4 Agnostic inference

Consistent estimation and variable selection inevitably depend on the existence of a “true” model. For sparse PCA, this corresponds to the assumption that the \( k \)-dimensional principal subspace of \( \Sigma \) is (1) identifiable and (2) sparse. Under this assumption, previous work [e.g. Vu+13] and the theory presented in Section 3 establish conditions under which consistent estimation and variable selection are possible. While these results can provide useful insights for sparse PCA and FPS, the conditions may or may not hold in practice. Therefore, it is important to understand the statistical inference problem without these assumptions. This is the agnostic inference perspective. Can we remove the assumptions of identifiability and sparsity? Is there an assumption-free interpretation for FPS?

Without assuming identifiability, variable selection and estimation consistency are no longer valid objectives, since there is no unique “true” parameter to estimate. For example, when \( \Sigma = I \), every \( k \)-dimensional subspace is a principal subspace, and even if there is a unique
principal subspace, it may not be sparse. To develop an assumption-free interpretation, we return to the basic objective function of PCA. Let $X$ be a random vector with covariance matrix $\Sigma$. PCA can be interpreted as a covariance maximization technique \cite{Vu+14}. It seeks a rank-$k$ projector $H$ that maximizes the predictive covariance:

$$\text{trace}(\text{Cov}(X, HX)) = \langle \Sigma, H \rangle.$$ 

We can interpret $H$ as a dimension reducing transformation and so $\langle \Sigma, H \rangle$ is just the total covariance between the input $X$ and output $HX$.

FPS also maximizes covariance, but it replaces the rank-$k$ constraint on $H$ with a Fantope constraint and an additional sparsity constraint via the $(1,1)$-norm. Let $\hat{H} := \arg\max_{H \in \mathcal{F}_k, \|H\|_{1,1} \leq R} \langle S, H \rangle.$ (11)

By Lagrangian duality, this constrained form of FPS is equivalent to the penalized form (2) in the sense that given $S$, for every $R$ there is a corresponding $\rho$ such that a solution of (2) is also a solution of (11) and vice-versa.

Our main result in the assumption-free setting is an interpretation of the constrained form of FPS and its persistence under no assumptions on $\Sigma$.

**Theorem 4** (Persistence). Let $X, X_1, \ldots, X_n \in \mathbb{R}^p$ be i.i.d. random vectors that satisfy the hypotheses of Proposition 1 (i.e. $X$ is sub-Gaussian). Then with probability at least $1 - 2^{-p}$, the constrained FPS estimator defined in (11) satisfies

$$\text{trace}(\text{Cov}(X, \hat{H}X)) \geq \max_{H \in \mathcal{F}_k, \|H\|_{1,1} \leq R} \text{trace}(\text{Cov}(X, HX)) - cR\lambda_1 \sqrt{\frac{\log p}{n}},$$

where $c > 0$ is a constant.

**Proof of Theorem 4.** Let $H_R$ be any solution of

$$\max_{H \in \mathcal{F}_k, \|H\|_{1,1} \leq R} \text{trace}(\text{Cov}(X, HX)).$$

Then $0 \leq \langle -\Sigma, \hat{H} - H_R \rangle$, and (11) implies $0 \leq \langle S, \hat{H} - H_R \rangle$. Combining these two inequalities with the Hölder and triangle inequalities yields

$$0 \leq \langle \Sigma, H_R \rangle - \langle \Sigma, \hat{H} \rangle \leq \langle S - \Sigma, \hat{H} - H_R \rangle \leq 2R\|S - \Sigma\|_{\infty,\infty}.$$

Finally, invoke Proposition 1 to complete the proof.
Theorem 4 shows that the predictive covariance of FPS comes close to that of the best sparse $H$ in the Fantope. This is essentially an assumption-free interpretation, however the meaning of $H \in \mathcal{F}^k$ may be unclear since it is not necessarily a projector.

As a linear map $x \mapsto Hx$, an element $H$ of the Fantope acts nearly like a rank-$k$ projector. There are two properties that characterize $H$. The first is $\text{trace}(H) = k$, which is like a degrees of freedom constraint for linear smoothers, in the sense that

$$\text{trace}(\text{Cov}(\xi, H\xi)) = k \text{ if } \text{Var}(\xi) = I.$$ 

The second characterizing property of $H$ is $0 \preceq H \preceq I$, which has several equivalent interpretations provided by the following Lemma.

**Lemma 4.** Let $H$ be a symmetric matrix. Then the following are equivalent.

1. $0 \preceq H \preceq I$.
2. $x \mapsto Hx$ is firmly non-expansive, i.e. $\|Hx - Hy\|_2^2 \leq \langle x - y, Hx - Hy \rangle$ for all $x, y$.
3. $\|x\|_2^2 \geq \|Hx\|_2^2 + \|(I - H)x\|_2^2$ for all $x$.
4. $\langle Hx, (I - H)x \rangle \geq 0$ for all $x$.

The proof is elementary and omitted.

5 Proofs of main sparsistency results

5.1 Proof of Theorem 2

5.1.1 Existence of a sparse solution

The primal dual witness argument starts from the dual form of the FPS problem (2). Using strong duality, we can write (2) in an equivalent min-max form.

$$\max_{H \in \mathcal{F}^k} \min_{Z \in \mathbb{B}_p} \langle S, H \rangle - \rho \langle H, Z \rangle,$$

$\Leftrightarrow \max_{H \in \mathcal{F}^k} \min_{Z \in \mathbb{B}_p} \langle S - \rho Z, H \rangle,$

(12)

$\Leftrightarrow \min_{Z \in \mathbb{B}_p} \max_{H \in \mathcal{F}^k} \langle S - \rho Z, H \rangle,$

(13)

where $\mathbb{B}_p = \{ Z \in \mathbb{R}^{p \times p} : \text{diag}(Z) = 0, Z = Z^T, \|Z\|_{\infty, \infty} \leq 1 \}$. According to the standard Karush-Kuhn-Tucker (KKT) condition, a pair $(\tilde{H}, \tilde{Z}) \in \mathcal{F}^k \times \mathbb{B}_p$ is optimal for problems
\( \hat{Z}_{ij} = \text{sign}(\hat{H}_{ij}) \quad \forall \ i \neq j, \ \hat{H}_{ij} \neq 0, \) \quad (14)\\
\hat{Z}_{ij} \in [-1, 1] \quad \forall \ i \neq j, \ \hat{H}_{ij} = 0, \) \quad (15)\\
\hat{H} = \arg \max_{H \in \mathcal{F}^k} \langle S - \rho Z, H \rangle. \) \quad (16)

To proceed with the primal dual witness argument, we first construct an additionally constrained solution \( \tilde{H} \) as follows.

\[ \tilde{H} = \arg \max_{H \in \mathcal{F}^k, \text{supp(diag}(H)) \subseteq J} \langle S, H \rangle - \rho \|H\|_{1,1}. \] \quad (17)

Denote \( \tilde{Z} \) the corresponding optimal dual variable. By Lemma 5, \( \tilde{H} \) is a rank-\( k \) projector supported on \( J \).

Let \( \begin{pmatrix} \hat{U}_J & 0 \end{pmatrix} \) and \( \begin{pmatrix} U_J & 0 \end{pmatrix} \) be \( p \times k \) orthogonal matrices consisting of the \( k \) leading eigenvectors of \( S - \rho \tilde{Z} \) and \( \Sigma \), respectively, where \( \hat{U}_J \) and \( U_J \) are \( s \times k \) orthogonal matrices.

According to Lemma 5, there exists a \( s \times s \) orthonormal matrix \( Q \) such that \( \hat{U}_J = QU_J \) and \( \|Q - I\|_F \leq 8 \rho s / (\lambda_k - \lambda_{k+1}) \).

Define the modified primal-dual pair \( (\tilde{H}, \tilde{Z}) \) as follows (recall that \( W = S - \Sigma \)).

\[ \tilde{H} = \tilde{H}, \]
\[ \tilde{Z}_{JJ} = \tilde{Z}_{JJ}, \] \quad (18)\\
\[ \tilde{Z}_{ij} = \frac{1}{\rho} \left\{ S_{ij} - \langle Q_{i*}, \Sigma_{J,j} \rangle \right\} \quad (i, j) \in J \times J^c, \] \quad (19)\\
\[ \tilde{Z}_{ij} = \frac{1}{\rho} W_{ij} \quad (i, j) \in (J^c)^2, \ i \neq j. \] \quad (20)

We need to check that \( (\tilde{H}, \tilde{Z}) \) are feasible for \( (12) \) and \( (13) \), and satisfy KKT conditions \( (14) \) to \( (16) \).

**Checking feasibility.** The feasibility of \( \tilde{H} \) is obvious. To check feasibility of \( \tilde{Z} \) we only need to verify that \( \tilde{Z}_{ij} \in [-1, 1] \) for all \( (i, j) \in J \times J^c \). In fact,

\[
|\tilde{Z}_{ij}| \leq \frac{1}{\rho} \left[ \|S_{ij} - \Sigma_{ij}\| + \|\Sigma_{ij} - \langle Q_{i*}, \Sigma_{J,j} \rangle\| \right] \leq \frac{1}{\rho} \left[ \|W\|_{\infty,\infty} + \|(I - Q)_{i*}\| \times \|\Sigma_{J,j}\| \right] \\
\leq \frac{1}{\rho} \left[ \|W\|_{\infty,\infty} + \|I - Q\|_F \|\Sigma_{J,J}\|_{2,\infty} \right] \leq \frac{\rho}{\rho} \left[ \|W\|_{\infty,\infty} + \frac{8 \rho s}{\lambda_k - \lambda_{k+1}} \|\Sigma_{J,J}\|_{2,\infty} \right] \\
\leq 1,
\]
where the last inequality follows from (7).

**Checking KKT condition (14).** Because \( \hat{H} \) only has non-zero entries in \( J \times J \), so \( (\hat{H}, \hat{Z}) \) satisfies (14) by construction.

**Checking KKT condition (15).** For \((i, j)\) in \( J \times J \), (15) is satisfied for \((\hat{H}, \hat{Z})\) because the same condition is satisfied for \((\tilde{H}, \tilde{Z})\). For \((i, j) \notin J \times J\), we have \( \hat{H}_{ij} = 0 \) and (15) follows from the feasibility of \( \hat{Z} \).

**Checking KKT condition (16).** Recall that \( W = S - \Sigma \). Let \( \tilde{W} \) be the \((p - s) \times (p - s)\) diagonal matrix that agrees with \( W_{Jc,Jc} \) on diagonal entries. By Lemma 1, it suffices to show that \( \left( \tilde{U}_J \right) \) spans a \( k \) dimensional principal subspace of

\[
\Sigma := S - \rho \tilde{Z} = \begin{pmatrix} S_{JJ} - \rho \tilde{Z}_{JJ} & Q \Sigma_{Jc,Jc} \\ \Sigma_{Jc,Jc} Q^T & \tilde{W} + \Sigma_{Jc,Jc} \end{pmatrix},
\]

which is established in Lemma 6.

Now we have shown that \((\tilde{H}, \tilde{Z})\) is indeed an optimal primal-dual pair for (12) and (13), and hence \( \hat{H} \) is a solution of (2) and is also supported only on \( J \).

### 5.1.2 Uniqueness of solution

Consider the elastic net version of FPS in (3) and its max-min and min-max forms using dual variable \( Z \in \mathbb{B}_p := \{ Z \in \mathbb{R}^{p \times p} : \text{diag}(Z) = 0, Z = Z^T, \| Z \|_{\infty, \infty} \leq 1 \} \):

\[
\min_{H \in \mathcal{F}^d} \max_{Z \in \mathbb{B}_p} -\langle S, H \rangle + \rho \langle H, Z \rangle + \frac{\tau}{2} \| H \|_F^2,
\]

\[
\iff \max_{Z \in \mathbb{B}_p} \min_{H \in \mathcal{F}^k} \frac{\tau}{2} \| H - \frac{1}{\tau} (S - \rho Z) \|_F^2 - \frac{1}{2\tau} \| S - \rho Z \|_F^2.
\]

The KKT condition for optimality of \((\tilde{H}, \tilde{Z}) \in \mathcal{F}^k \times \mathbb{B}_p\) becomes

\[
\tilde{Z}_{ij} = \text{sign}(\tilde{H}_{ij}) \quad \forall \ i \neq j, \ \tilde{H}_{ij} \neq 0,
\]

\[
\tilde{Z}_{ij} \in [-1,1] \quad \forall \ i \neq j, \ \tilde{H}_{ij} = 0,
\]

\[
\tilde{H} = \mathcal{P}_{\mathcal{F}^k} \left( \frac{1}{\tau} (S - \rho \tilde{Z}) \right).
\]

Let \( \tilde{H}, \tilde{Z} \) be the support constrained FPS solution in (17) and \( \tilde{Z} \) be the dual variable constructed in (18) to (20). We first show that \((\tilde{H}, \tilde{Z})\) is also optimal for the elastic net version of FPS when \( \tau \) is small enough.
From the existence proof above and Lemma 6 we know that (i) \( S - \rho \hat{Z} = \tilde{\Sigma} \); (ii) the \( k \) dimensional principal subspace of \( \tilde{\Sigma} \) is spanned by \( \begin{pmatrix} \hat{U}_J \\ 0 \end{pmatrix} \); and (iii) \( \lambda_k(\tilde{\Sigma}) - \lambda_{k+1}(\tilde{\Sigma}) > 0 \).

By the construction of \( \tilde{H} \), part 3 of Lemma 1 implies that, when

\[
0 < \tau \leq \lambda_k(\tilde{\Sigma}) - \lambda_{k+1}(\tilde{\Sigma})
\]

we have

\[
\tilde{H} = \mathcal{P}_{\mathcal{F}^k} \left( \frac{1}{\tau} \left( S - \rho \hat{Z} \right) \right).
\]

As a consequence, \((\tilde{H}, \hat{Z})\) is also an optimal primal-dual pair for the elastic net FPS problem (3) when \( \tau \) is in the range specified in (25).

Now we prove uniqueness of \( \tilde{H} \) as a solution to the FPS problem (2). Assume that there is another solution \( \tilde{H}' \in \mathcal{F}^k \) such that

\[
\langle S, \tilde{H} \rangle - \rho \| \tilde{H} \|_{1,1} = \langle S, \tilde{H}' \rangle - \rho \| \tilde{H}' \|_{1,1}.
\]

But \( \tilde{H} \) is the unique solution to the elastic net FPS for \( \tau > 0 \) small enough, we must have \( \| \tilde{H}' \|_F^2 > \| \tilde{H} \|_F^2 \) and hence

\[
k \geq \| \tilde{H}' \|_F^2 > \| \tilde{H} \|_F^2 = k,
\]

which is a contradiction (the first inequality follows from that \( \tilde{H}' \in \mathcal{F}^k \)).

**5.2 Auxiliary Lemmas**

**Lemma 5.** Under the assumptions in Theorem 2, let \( \tilde{H} \) be the solution to the further constrained problem (17). Then \( \tilde{H} \) is rank \( k \) and unique. Furthermore, there exist \( s \times k \) orthonormal matrices \( U_J, \hat{U}_J \) such that

1. \( \begin{pmatrix} U_J \\ 0 \end{pmatrix} \) and \( \begin{pmatrix} \hat{U}_J \\ 0 \end{pmatrix} \) span the \( k \) dimensional principal subspaces of \( \Sigma \) and \( S - \rho \hat{Z} \) respectively.

2. There exists a \( s \times s \) orthonormal matrix \( Q \) such that

\[
\hat{U}_J = Q U_J,
\]

\[
\| Q - I \|_F \leq \frac{8 \rho s}{\lambda_k - \lambda_{k+1}}.
\]
Therefore, the above two inequalities jointly imply that
\[
\lambda_k(\tilde{\Sigma}_{1J}) - \lambda_{k+1}(\tilde{\Sigma}_{1J}) \geq \lambda_k(\Sigma_{1J}) - \lambda_{k+1}(\Sigma_{1J}) - 4\rho_s \geq \lambda_k - \lambda_{k+1} - 4\rho_s > 0
\]
by condition (8). The first claim follows from part 1 of Lemma 1.

The second claim is trivial when \( s = k \). Now we focus on the case \( s > k \). By the SPS condition we know that the unique \( k \) dimensional principal subspace of \( \Sigma \) is spanned by the columns of \( \tilde{U}_J \) and \( U_J \) spans the \( k \) dimensional principal subspace of \( \Sigma_{1J} \).

Using the fact that \( \lambda_k(\Sigma_{1J}) - \lambda_{k+1}(\Sigma_{1J}) \geq \lambda_k - \lambda_{k+1} \), and applying Proposition 2.2 in [VL13], we can choose the right rotations for the columns of \( \tilde{U}_J, U_J \) so that
\[
\|\tilde{U}_J - U_J\|_F \leq \|\tilde{U}_J \tilde{U}_J^T - U_J U_J^T\|_F.
\]
Using Lemma 4.2 of [VL13] and Cauchy-Schwartz we have
\[
\|\tilde{U}_J \tilde{U}_J^T - U_J U_J^T\|_F \leq \frac{2}{\lambda_k - \lambda_{k+1}} \|\tilde{\Sigma}_{1J} - \Sigma_{1J}\|_F \leq \frac{4\rho_s}{\lambda_k - \lambda_{k+1}}.
\]
The above two inequalities jointly imply that
\[
\|\tilde{U}_J - U_J\|_F \leq \frac{4\rho_s}{\lambda_k - \lambda_{k+1}}.
\]
Now let \( \tilde{V} = (\tilde{U}_J, \tilde{U}_J^c) \) be an \( s \times s \) orthonormal matrix, and similarly \( V = (U_J, U_J^c) \). One can show that, using the same argument as above, \( \tilde{U}_J^c \) and \( U_J^c \) can be chosen such that
\[
\|\tilde{U}_J^c - U_J^c\|_F \leq \frac{4\rho_s}{\lambda_k - \lambda_{k+1}}.
\]
Let \( Q = \tilde{V} V^T \), then \( \tilde{Q} U_J = \tilde{U}_J \) and
\[
\|I - Q\|_F = \|(V - \tilde{V})V^T\|_F = \|\tilde{V} - V\|_F \leq \frac{8\rho_s}{\lambda_k - \lambda_{k+1}}.
\]

**Lemma 6.** Under the assumptions of Theorem 2, let \( (\tilde{H}, \tilde{Z}) \) be the optimal primal-dual pair of the additionally constrained FPS problem (17). Let \( \left( \tilde{U}_J, 0 \right) \), \( \left( U_J, 0 \right) \), and \( Q \) be defined as in Lemma 5. Let \( \tilde{\Sigma} \) be defined as in (21). Then
\[
\lambda_k(\tilde{\Sigma}) - \lambda_{k+1}(\tilde{\Sigma}) > 0
\]
and \( \tilde{H} \) is the unique projector of the the \( k \)-dimensional principal subspace of \( \tilde{\Sigma} \).
Proof. We start from a decomposition of $\tilde{\Sigma}$ as follows.

$$
\tilde{\Sigma} = \begin{pmatrix}
S_{JJ} - \rho \tilde{Z}_{JJ} & Q\Sigma_{JJc} \\
\Sigma_{Jc}Q^T & \tilde{W} + \Sigma_{JcJc}
\end{pmatrix}
$$

$$
= \begin{pmatrix}
S_{JJ} - \rho \tilde{Z}_{JJ} - Q\Sigma_{JJ}Q^T + Q\Sigma_{JJ}Q^T & Q\Sigma_{JJc} \\
\Sigma_{Jc}Q^T & \tilde{W} + \Sigma_{JcJc}
\end{pmatrix}
$$

$$
= \begin{pmatrix}
S_{JJ} - \rho \tilde{Z}_{JJ} - Q\Sigma_{JJ}Q^T & 0 \\
0 & \tilde{W}
\end{pmatrix} + \begin{pmatrix}
Q\Sigma_{JJ}Q^T & Q\Sigma_{JJc} \\
\Sigma_{Jc}Q^T & \Sigma_{JcJc}
\end{pmatrix}
$$

= "noise" + "signal".

(26)

It can be directly verified that $\begin{pmatrix}
\hat{U}_{J0} \\
0
\end{pmatrix}$ spans the $d$-principal subspace of $\begin{pmatrix}
Q\Sigma_{JJ}Q^T & Q\Sigma_{JJc} \\
\Sigma_{Jc}Q^T & \Sigma_{JcJc}
\end{pmatrix} = \begin{pmatrix}
Q & 0 \\
0 & I
\end{pmatrix} \times \Sigma \times \begin{pmatrix}
Q^T & 0 \\
0 & I
\end{pmatrix}.$

(27)

Moreover, (27) implies that the eigenvalues of the "signal" part in the decomposition (26) are the same as those of $\Sigma$.

To sum up, we have so far shown that $\begin{pmatrix}
\hat{U}_{J0} \\
0
\end{pmatrix}$ spans the $k$-dimensional principal subspace of the signal part, with eigengap $\lambda_k - \lambda_{k+1}$.

Next we need to show that the $k$ dimensional principal subspace remains unchanged after adding the "noise" part.

First, the block-diagonal structure of the "noise" matrix in (26) ensures that $\begin{pmatrix}
\hat{U}_{J0} \\
0
\end{pmatrix}$ spans one of its $k$-dimensional spectral subspace (a $k$ dimensional spectral subspace of a $p \times p$ symmetric matrix $A$ means that if $v$ is in this subspace, then $Av$ is also in this subspace).

Second, we show that twice the operator norm of the "noise" part is smaller than the gap between $k$th and $(k+1)$th eigenvalues of $\tilde{\Sigma}$, which is $\lambda_k - \lambda_{k+1}$. In fact, the operator norm of the noise part does not exceed

$$
\|S_{JJ} - \rho \tilde{Z}_{JJ} - \Sigma_{JJ}\| + \|\Sigma_{JJ} - Q\Sigma_{JJ}Q^T\| \leq 2\rho s + 2\|\Sigma_{JJ}\| \times \|Q - I\| \\
\leq 2\rho s + 2\lambda_1 \times 8\rho s/(\lambda_k - \lambda_{k+1}),
$$

where the bound on $\|Q - I\|$ comes from Lemma 5. We also have $\|\tilde{W}\| \leq \rho$, which is contained within the above bound.

Therefore, by standard perturbation theory such as Weyl’s inequality, the subspace spanned by $\begin{pmatrix}
\hat{U}_{J0} \\
0
\end{pmatrix}$ is the $k$ dimensional principal subspace of $\tilde{\Sigma}$ as long as

$$
4\rho s + 16\sqrt{2}\lambda_1 \rho s/(\lambda_k - \lambda_{k+1}) \leq \lambda_k - \lambda_{k+1},
$$

(28)
which means that twice the noise operator norm does not exceed the spectral gap in the signal part.

When the inequality in (28) is strict, as stated in condition (8), we know that the $k$-dimensional principal subspace of $\tilde{\Sigma}$ is unique. ■

6 Discussion

A connection between sparse PCA and sparse linear regression has been observed by Vu and Lei [VL13]. They established minimax rates for estimation under $\ell_2$ loss with $\ell_q$-penalized estimators with suitably defined model parameters and observed that the rates are identical to those for sparse linear regression when the effective noise variance is defined appropriately. The sparsistency result in the present paper further extends this connection to variable selection. Roughly speaking, the previously used spiked covariance model in sparse PCA, which assumes that

$$\Sigma = U \Lambda U^T + \sigma^2 I_p,$$

where $U$ is $p \times k$ orthonormal matrix and $\Lambda \succ 0$ is diagonal [see, e.g., Bir+13; CMW13; JL09; Ma13], corresponds to the orthogonal design in linear regression, in the sense that the relevant and noise variables are not correlated. Moreover, the $\sigma^2 I$ term boosts the signal by adding $\sigma^2$ to all the relevant diagonal entries in $\Sigma$, and therefore, thresholding based methods usually work well. The limited correlation condition developed in this paper is analogous to the irrepresentable condition or mutual incoherence condition [MB06; ZY06] for the $\ell_1$ penalized sparse regression (LASSO), where convex optimization methods can succeed when the correlation between relevant and noise variables is small.

When the eigenvalues of $\Sigma$ are fixed, a sufficient condition for consistent variable selection using FPS is $s \lesssim \sqrt{n/\log p}$. This is comparable to the corresponding rate developed for $k = 1$ by Amini and Wainwright [AW09] when the rank of the solution is not assumed to be 1. It has been shown by Amini and Wainwright [AW09] that the information-theoretic critical rate is $s \lesssim n/\log p$. That is, if $s \gg n/\log p$, no method can succeed in variable selection. It remains an open question if there exist polynomial time methods that can consistently select relevant variables in the range $\sqrt{n/\log p} \lesssim s \lesssim n/\log p$. An interesting work in this direction is that by Berthet and Rigollet [BR13a], which shows that, for $k = 1$, testing a sparse PCA model in this regime is at least as hard as solving the planted clique problem beyond the well-believed computational barrier. We believe that the same scheme can be applied to variable selection and will pursue this idea in a future work.

The predictive covariance maximization interpretation of PCA leads to a natural characterization of the Fantope as the collection of all symmetric firmly non-expansive linear transformations with $k$ degrees of freedom. Without any assumptions on $\Sigma$, FPS gives us
a dimension reducing transformation that is sparse while being computationally tractable, and it nearly approaches the best predictive covariance. In practice, it would be suitable to estimate the predictive covariance of the FPS solution for a particular value of $\rho$ using risk estimates such as cross-validation. This leads to a data-driven procedure for selecting the best FPS tuning parameter $\rho$. The detailed design and properties of such a cross-validation method is an important and interesting topic for future work.

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