

Sparse PCA via Bipartite Matchings

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Abstract

We consider the following multi-component sparse PCA problem: given a set of data points, we seek to extract a small number of sparse components with *disjoint* supports that jointly capture the maximum possible variance. These components can be computed one by one, repeatedly solving the single-component problem and deflating the input data matrix, but as we show this greedy procedure is suboptimal. We present a novel algorithm for sparse PCA that jointly optimizes multiple disjoint components. The extracted features capture variance that lies within a multiplicative factor arbitrarily close to 1 from the optimal. Our algorithm is combinatorial and computes the desired components by solving multiple instances of the bipartite maximum weight matching problem. Its complexity grows as a low order polynomial in the ambient dimension of the input data matrix, but exponentially in its rank. However, it can be effectively applied on a low-dimensional sketch of the data; this allows us to obtain polynomial-time approximation guarantees via spectral bounds. We evaluate our algorithm on real data-sets and empirically demonstrate that in many cases it outperforms existing, deflation-based approaches.

1 Introduction

Principal Component Analysis (PCA) reduces the dimensionality of a data set by projecting it onto principal subspaces spanned by the leading eigenvectors of the sample covariance matrix. Sparse PCA is a useful variant that offers higher data interpretability [1, 2, 3], a property that is sometimes desired even at the cost of statistical fidelity [4]. Furthermore, when the obtained features are used in subsequent learning tasks, sparsity potentially leads to better generalization error [5].

Given a real $n \times d$ data matrix \mathbf{S} representing n centered data points supported on d features, the leading sparse principal component of the data set is the sparse vector that maximizes the explained variance:

$$\mathbf{x}_\star \triangleq \arg \max_{\|\mathbf{x}\|_2=1, \|\mathbf{x}\|_0=s} \mathbf{x}^\top \mathbf{A} \mathbf{x}, \quad (1)$$

where $\mathbf{A} = 1/n \cdot \mathbf{S}^\top \mathbf{S}$ is the $d \times d$ empirical covariance matrix. The sparsity constraint makes the problem NP-hard and hence computationally intractable in general, and hard to approximate within some small constant [6]. A significant volume of prior work has focused on algorithms that approximately solve the optimization problem [2, 3, 4, 7, 8, 9, 10, 11, 12, 13, 14, 15], while a large volume of theoretical results has been established under planted statistical models [16, 17, 18, 19, 20, 21, 22, 23, 24].

In most practical settings, we tend to go beyond computing a single sparse PC. Contrary to the single-component problem, there has been limited work on computing multiple components. The scarcity is partially attributed to conventional PCA wisdom: multiple components can be computed one-by-one, repeatedly, by solving the single-component sparse PCA problem (1) and *deflating* the input data to remove information captured by previously extracted components [25]. In fact, the multi-component version of sparse PCA is not uniquely defined in the literature. Different deflation-based approaches can lead to different outputs: extracted components may or may not be orthogonal, while they may have disjoint or overlapping supports [25]. In the statistics literature, where the objective is typically to recover a “true” principal subspace, a branch of work has focused on the “subspace row sparsity” [26], an assumption that leads to sparse components all supported on the same set of variables. While in [27], the authors discuss an alternative perspective on the fundamental objective of the sparse PCA problem.

In this work, we develop a novel algorithm for the multi-component sparse PCA problem with disjoint supports. Formally, we are interested in finding k components that are s -sparse, have disjoint supports, and jointly maximize the explained variance:

$$\mathbf{X}_* \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}_k} \text{Tr}(\mathbf{X}^\top \mathbf{A} \mathbf{X}), \quad (2)$$

where the feasible set is

$$\mathcal{X}_k \triangleq \{\mathbf{X} \in \mathbb{R}^{d \times k} : \|\mathbf{X}^j\|_2 = 1, \|\mathbf{X}^j\|_0 = s, \text{supp}(\mathbf{X}^i) \cap \text{supp}(\mathbf{X}^j) = \emptyset, \forall j \in [k], i < j\},$$

with \mathbf{X}^j denoting the j th column of \mathbf{X} . The number k of the desired components is a user defined parameter and we consider it to be a small constant.

Contrary to the greedy sequential approach that repeatedly uses deflation, our algorithm *jointly* computes all the vectors in \mathbf{X} , and comes with theoretical approximation guarantees. We note that even if one could solve each single-component sparse PCA problem (1) *exactly*, greedy deflation can be highly suboptimal. We show this through a simple example in Section 7.

Our Contributions

1. We develop an algorithm that provably approximates the solution to the sparse PCA problem (2) within a multiplicative factor arbitrarily close to 1. To the best of our knowledge, this is the first algorithm that jointly optimizes multiple components with disjoint supports, provably. Our algorithm is combinatorial; it recasts sparse PCA as multiple instances of *bipartite maximum weight matching* on graphs determined by the input data.
2. The computational complexity of our algorithm grows as a low order polynomial in the ambient dimension d , but is exponential in the intrinsic dimension of the input data, *i.e.*, the rank of \mathbf{A} . To alleviate the impact of this dependence, our algorithm can be applied on a low-dimensional sketch of the input data to obtain an approximate solution to (2). This extra level of approximation introduces an additional penalty in our theoretical approximation guarantees, which naturally depends on the quality of the sketch and, in turn, the spectral decay of \mathbf{A} . We show how these bounds further translate to an additive PTAS (polynomial-time approximation scheme) for sparse PCA. Our additive PTAS outputs an approximate solution with explained variance of at least $\text{OPT} - \epsilon \cdot s$, for any sparsity $s \in \{1, \dots, n\}$, any constant error $\epsilon > 0$ and any $k = O(1)$ number of orthogonal components.¹

¹Here, OPT is the explained variance captured by the optimal set of k components that are s sparse and have disjoint supports.

3. We empirically evaluate our algorithm on real datasets, and compare it against state-of-the-art methods for the single-component sparse PCA problem (1) in conjunction with the appropriate deflation step. In many cases, our algorithm—as a result of jointly optimizing over multiple components—leads to significantly improved results, and outperforms deflation-based approaches.

2 Sparse PCA through Bipartite Matchings

Our algorithm approximately solves the constrained maximization (2) on a $d \times d$ rank- r PSD matrix \mathbf{A} within a multiplicative factor arbitrarily close to 1. It operates by recasting the maximization into multiple instances of the bipartite maximum weight matching problem. Each instance ultimately yields a feasible solution: a set of k components that are s -sparse and have disjoint supports. The algorithm examines these solutions, and outputs the one that maximizes the explained variance, *i.e.*, the quadratic objective in (2).

The computational complexity of our algorithm grows as a low order polynomial in the ambient dimension d of the input, but exponentially in its rank r . Despite the unfavorable dependence on the rank, it is unlikely that a substantial improvement can be achieved in general [6]. However, decoupling the dependence on the ambient and the intrinsic dimension of the input has an interesting ramification; instead of the original input \mathbf{A} , our algorithm can be applied on a low-rank surrogate to obtain an approximate solution, alleviating the dependence on r . We discuss this in Section 3, and present the approximation bound that this allows us to obtain.

Let $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$ denote the truncated eigenvalue decomposition of \mathbf{A} ; $\mathbf{\Lambda}$ is a diagonal $r \times r$ whose i th diagonal entry is equal to the i th largest eigenvalue of \mathbf{A} , while the columns of \mathbf{U} are the corresponding eigenvectors. By the Cauchy-Schwartz inequality, for any $\mathbf{x} \in \mathbb{R}^d$,

$$\mathbf{x}^\top \mathbf{A} \mathbf{x} = \|\mathbf{\Lambda}^{1/2} \mathbf{U}^\top \mathbf{x}\|_2^2 \geq \langle \mathbf{\Lambda}^{1/2} \mathbf{U}^\top \mathbf{x}, \mathbf{c} \rangle^2, \quad \forall \mathbf{c} \in \mathbb{R}^r : \|\mathbf{c}\|_2 = 1. \quad (3)$$

In fact, equality in (3) can always be achieved for \mathbf{c} colinear to $\mathbf{\Lambda}^{1/2} \mathbf{U}^\top \mathbf{x} \in \mathbb{R}^r$ and in turn

$$\mathbf{x}^\top \mathbf{A} \mathbf{x} = \max_{\mathbf{c} \in \mathbb{S}_2^{r-1}} \langle \mathbf{x}, \mathbf{U} \mathbf{\Lambda}^{1/2} \mathbf{c} \rangle^2,$$

where \mathbb{S}_2^{r-1} denotes the ℓ_2 -unit sphere in r dimensions. More generally, for any $\mathbf{X} \in \mathbb{R}^{d \times k}$,

$$\text{Tr}(\mathbf{X}^\top \mathbf{A} \mathbf{X}) = \sum_{j=1}^k \mathbf{X}^j \mathbf{X}^j \mathbf{A} \mathbf{X}^j = \max_{\mathbf{C}: \mathbf{C}^j \in \mathbb{S}_2^{r-1} \forall j} \sum_{j=1}^k \langle \mathbf{X}^j, \mathbf{U} \mathbf{\Lambda}^{1/2} \mathbf{C}^j \rangle^2. \quad (4)$$

Under the variational characterization of the trace objective in (4), the sparse PCA problem (2) can be re-written as a joint maximization over the variables \mathbf{X} and \mathbf{C} as follows:

$$\max_{\mathbf{X} \in \mathcal{X}_k} \text{Tr}(\mathbf{X}^\top \mathbf{A} \mathbf{X}) = \max_{\mathbf{X} \in \mathcal{X}_k} \max_{\mathbf{C}: \mathbf{C}^j \in \mathbb{S}_2^{r-1} \forall j} \sum_{j=1}^k \langle \mathbf{X}^j, \mathbf{U} \mathbf{\Lambda}^{1/2} \mathbf{C}^j \rangle^2. \quad (5)$$

The alternative formulation of the sparse PCA problem in (5) takes a step towards decoupling the dependence of the optimization on the ambient and intrinsic dimensions d and r , respectively. The motivation behind the introduction of the auxiliary variable \mathbf{C} will become clear in the sequel.

For a given \mathbf{C} , the value of $\mathbf{X} \in \mathcal{X}_k$ that maximizes the objective in (5) for that \mathbf{C} is

$$\widehat{\mathbf{X}} \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}_k} \sum_{j=1}^k \langle \mathbf{X}^j, \mathbf{W}^j \rangle^2, \quad (6)$$

where $\mathbf{W} \triangleq \mathbf{U}\mathbf{\Lambda}^{1/2}\mathbf{C}$ is a real $d \times k$ matrix. The constrained, non-convex maximization (6) plays a central role in our developments. We will later describe a combinatorial $O(d \cdot (s \cdot k)^2)$ procedure to efficiently compute $\widehat{\mathbf{X}}$, reducing the maximization to an instance of the bipartite maximum weight matching problem. For now, however, let us assume that such a procedure exists.

Let \mathbf{X}_* , \mathbf{C}_* be the pair that attains the maximum in (5); in other words, \mathbf{X}_* is the desired solution to the sparse PCA problem. If the optimal auxiliary variable \mathbf{C}_* was known, then we would be able to recover \mathbf{X}_* by solving the maximization (6) for $\mathbf{C} = \mathbf{C}_*$. Of course, \mathbf{C}_* is not known, and it is not possible to exhaustively consider all possible values in the domain of \mathbf{C} . Instead, we examine only a finite number of possible values of \mathbf{C} over a fine discretization of its domain. In particular, let $\mathcal{N}_{\epsilon/2}(\mathbb{S}_2^{r-1})$ denote a finite $\epsilon/2$ -net of the r -dimensional ℓ_2 -unit sphere; for any point in \mathbb{S}_2^{r-1} , the net contains a point within an $\epsilon/2$ radius from the former. There are several ways to construct such a net [28]. Further, let $[\mathcal{N}_{\epsilon/2}(\mathbb{S}_2^{r-1})]^{\otimes k} \subset \mathbb{R}^{d \times k}$ denote the k th Cartesian power of the aforementioned $\epsilon/2$ -net. By construction, this collection of points contains a matrix \mathbf{C} that is column-wise close to \mathbf{C}_* . In turn, it can be shown using the properties of the net, that the candidate solution $\mathbf{X} \in \mathcal{X}_k$ obtained through (6) at that point \mathbf{C} will be approximately as good as the optimal \mathbf{X}_* in terms of the quadratic objective in (2).

All above observations yield a procedure for approximately solving the sparse PCA problem (2). The steps are outlined in Algorithm 1. Given the desired number of components k and an accuracy parameter $\epsilon \in (0, 1)$, the algorithm generates a net $[\mathcal{N}_{\epsilon/2}(\mathbb{S}_2^{r-1})]^{\otimes k}$ and iterates over its points. At each point \mathbf{C} , it computes a feasible solution for the sparse PCA problem – a set of k s -sparse components – by solving the maximization in (6) via a procedure (Alg. 2) that will be described in the sequel. The algorithm collects the candidate solutions identified at the points of the net. The best among them achieves an objective in (2) that provably lies close to optimal. More formally,

Algorithm 1 Sparse PCA (Multiple disjoint components)

input : PSD $d \times d$ rank- r matrix \mathbf{A} , $\epsilon \in (0, 1)$, $k \in \mathbb{Z}_+$.
output : $\overline{\mathbf{X}} \in \mathcal{X}_k$ {Theorem 1}
1: $\mathcal{C} \leftarrow \{\}$
2: $[\mathbf{U}, \mathbf{\Lambda}] \leftarrow \text{EIG}(\mathbf{A})$
3: **for each** $\mathbf{C} \in [\mathcal{N}_{\epsilon/2}(\mathbb{S}_2^{r-1})]^{\otimes k}$ **do**
4: $\mathbf{W} \leftarrow \mathbf{U}\mathbf{\Lambda}^{1/2}\mathbf{C}$ { $\mathbf{W} \in \mathbb{R}^{d \times k}$ }
5: $\widehat{\mathbf{X}} \leftarrow \arg \max_{\mathbf{X} \in \mathcal{X}_k} \sum_{j=1}^k \langle \mathbf{X}^j, \mathbf{W}^j \rangle^2$ {Alg. 2}
6: $\mathcal{C} \leftarrow \mathcal{C} \cup \{\widehat{\mathbf{X}}\}$
7: **end for**
8: $\overline{\mathbf{X}} \leftarrow \arg \max_{\mathbf{X} \in \mathcal{C}} \text{TR}(\mathbf{X}^\top \mathbf{A} \mathbf{X})$

Theorem 1. *For any real $d \times d$ rank- r PSD matrix \mathbf{A} , desired number of components k , number s of nonzero entries per component, and accuracy parameter $\epsilon \in (0, 1)$, Algorithm 1 outputs $\overline{\mathbf{X}} \in \mathcal{X}_k$ such that*

$$\text{TR}(\overline{\mathbf{X}}^\top \mathbf{A} \overline{\mathbf{X}}) \geq (1 - \epsilon) \cdot \text{TR}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*),$$

where $\mathbf{X}_* \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}_k} \text{TR}(\mathbf{X}^\top \mathbf{A} \mathbf{X})$, in time $T_{\text{SVD}}(r) + O\left(\left(\frac{4}{\epsilon}\right)^{r \cdot k} \cdot d \cdot (s \cdot k)^2\right)$.

Algorithm 1 is the first nontrivial algorithm that provably approximates the solution of the sparse PCA problem (2). According to Theorem 1, it achieves an objective value that lies within a multiplicative factor from the optimal, arbitrarily close to 1. Its complexity grows as a low-order polynomial in the dimension d of the input, but exponentially in the intrinsic dimension r . Note, however, that it can be exponentially faster compared to the $O(d^{s \cdot k})$ brute force approach that exhaustively considers all candidate supports for the k sparse components. The complexity of our algorithm follows from the cardinality of the net and the complexity of Algorithm 2, the subroutine that solves the constrained maximization (6). The latter is a key ingredient of our algorithm, and is discussed in detail in the next subsection. A formal proof of Theorem 1 is provided in Section 9.2.

2.1 Sparse Components via Bipartite Matchings

In the core of Algorithm 1 lies Algorithm 2, a procedure that solves the constrained maximization in (6). The algorithm breaks down the maximization into two stages. First, it identifies the support of the optimal solution $\widehat{\mathbf{X}}$. Determining the support reduces to an instance of the maximum matching problem on a weighted bipartite graph G . Then, it recovers the exact values of the nonzero entries in $\widehat{\mathbf{X}}$ based on the Cauchy-Schwarz inequality. In the sequel, we provide a brief description of Algorithm 2, leading up to its guarantees in Lemma 2.1.

Let $\mathcal{I}_j \triangleq \text{supp}(\widehat{\mathbf{X}}^j)$ be the support of the j th column of $\widehat{\mathbf{X}}$, $j = 1, \dots, k$. The objective in (6) becomes

$$\sum_{j=1}^k \langle \widehat{\mathbf{X}}^j, \mathbf{w}^j \rangle^2 = \sum_{j=1}^k \left(\sum_{i \in \mathcal{I}_j} \widehat{X}_{ij} \cdot W_{ij} \right)^2 \leq \sum_{j=1}^k \sum_{i \in \mathcal{I}_j} W_{ij}^2. \quad (7)$$

The last inequality is an application of the Cauchy-Schwarz Inequality and the constraint $\|\mathbf{X}^j\|_2 = 1 \forall j \in \{1, \dots, k\}$. In fact, if an oracle reveals the supports \mathcal{I}_j , $j = 1, \dots, k$, the upper bound in (7) can always be achieved by setting the nonzero entries of $\widehat{\mathbf{X}}$ as in Algorithm 2 (Line 6). Therefore, the key in solving (6) is determining the collection of supports to maximize the right-hand side of (7).

By constraint, the sets \mathcal{I}_j must be pairwise disjoint, each with cardinality s . Consider a weighted bipartite graph $G = (U = \{U_1, \dots, U_k\}, V, E)$ constructed as follows² (Fig. 1):

- V is a set of d vertices v_1, \dots, v_d , corresponding to the d variables, *i.e.*, the d rows of $\widehat{\mathbf{X}}$.
- U is a set of $k \cdot s$ vertices, conceptually partitioned into k disjoint subsets U_1, \dots, U_k , each of cardinality s . The j th subset, U_j , is associated with the support \mathcal{I}_j ; the s vertices $u_\alpha^{(j)}$, $\alpha = 1, \dots, s$ in U_j serve as placeholders for the variables/indices in \mathcal{I}_j .
- Finally, the edge set is $E = U \times V$. The edge weights are determined by the $d \times k$ matrix \mathbf{W} in (6). In particular, the weight of edge $(u_\alpha^{(j)}, v_i)$ is equal to W_{ij}^2 . Note that all vertices in U_j are effectively identical; they all share a common neighborhood and edge weights.

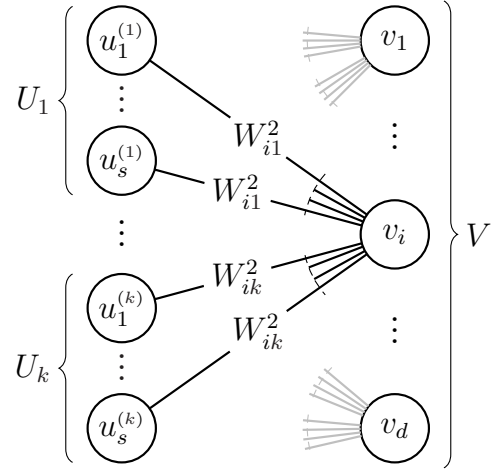


Figure 1: The graph G generated by Alg. 2. It is used to determine the support of the solution $\widehat{\mathbf{X}}$ in (6).

Any feasible support $\{\mathcal{I}_j\}_{j=1}^k$ corresponds to a *perfect matching* in G and vice-versa. Recall that a matching is a subset of the edges containing no two edges incident to the same vertex, while a perfect matching, in the case of an unbalanced bipartite graph $G = (U, V, E)$ with $|U| \leq |V|$, is a matching that contains at least one incident edge for each vertex in U . Given a perfect matching $\mathcal{M} \subseteq E$, the disjoint neighborhoods of U_j s under \mathcal{M} yield a support $\{\mathcal{I}_j\}_{j=1}^k$. Conversely, any valid support yields a unique perfect matching in G (taking into account that all vertices in U_j are isomorphic). Moreover, due to the choice of weights in G , the right-hand side of (7) for a given support $\{\mathcal{I}_j\}_{j=1}^k$ is equal to the weight of the matching \mathcal{M} in G induced by the former, *i.e.*,

²The construction is formally outlined in Algorithm 4 in Section 8.

Algorithm 2 Compute Candidate Solution

input Real $d \times k$ matrix \mathbf{W}

output $\hat{\mathbf{X}} = \arg \max_{\mathbf{X} \in \mathcal{X}_k} \sum_{j=1}^k \langle \mathbf{X}^j, \mathbf{W}^j \rangle^2$

1: $G(\{U_j\}_{j=1}^k, V, E) \leftarrow \text{GENBIGRAPH}(\mathbf{W})$ {Alg. 4}

2: $\mathcal{M} \leftarrow \text{MAXWEIGHTMATCH}(G)$ { $\subset E$ }

3: $\hat{\mathbf{X}} \leftarrow \mathbf{0}_{d \times k}$

4: **for** $j = 1, \dots, k$ **do**

5: $\mathcal{I}_j \leftarrow \{i \in \{1, \dots, d\} : (u, v_i) \in \mathcal{M}, u \in U_j\}$

6: $[\hat{\mathbf{X}}^j]_{\mathcal{I}_j} \leftarrow [\mathbf{W}^j]_{\mathcal{I}_j} / \|\mathbf{W}^j\|_2$

7: **end for**

$\sum_{j=1}^k \sum_{i \in \mathcal{I}_j} W_{ij}^2 = \sum_{(u,v) \in \mathcal{M}} w(u,v)$. It follows that *determining the support of the solution in (6), reduces to solving the maximum weight matching problem on the bipartite graph G .*

Algorithm 2 readily follows. Given $\mathbf{W} \in \mathbb{R}^{d \times k}$, the algorithm generates a weighted bipartite graph G as described, and computes its maximum weight matching. Based on the latter, it first recovers the desired support of $\hat{\mathbf{X}}$ (Line 5), and subsequently the exact values of its nonzero entries (Line 6). The running time is dominated by the computation of the matching, which can be done in $O(|E||U| + |U|^2 \log |U|)$ using a variant of the Hungarian algorithm [29]. Hence,

Lemma 2.1. *For any $\mathbf{W} \in \mathbb{R}^{d \times k}$, Algorithm 2 computes the solution to (6), in time $O(d \cdot (s \cdot k)^2)$.*

A more formal analysis and proof of Lemma 2.1 is available in Section 9.1. With Algorithm 2 and Lemma 2.1 in place, we complete the description of our sparse PCA algorithm (Algorithm 1) and the proof sketch of Theorem 1.

3 Sparse PCA on Low-Dimensional Sketches

Algorithm 1 approximately solves the sparse PCA problem (2) on a $d \times d$ rank- r PSD matrix \mathbf{A} , in time that grows as a low-order polynomial in the ambient dimension d , but depends exponentially on r . This dependence can be prohibitive in practice. To mitigate its effect, instead of the original input, we can apply our sparse PCA algorithm on a low-rank approximation of \mathbf{A} .

Intuitively, the quality of the extracted components should depend on how well that low-rank surrogate approximates the original input.

More formally, let \mathbf{S} be the real $n \times d$ data matrix representing n (potentially centered) datapoints in d variables, and \mathbf{A} the corresponding $d \times d$ covariance matrix. Further, let $\bar{\mathbf{S}}$ be a low-dimensional sketch of the original data; an $n \times d$ matrix whose rows lie in an r -dimensional subspace, with r being an accuracy parameter. Such a sketch can be obtained in several ways, including for example exact or approximate SVD, or online sketching methods [30]. Finally, let $\bar{\mathbf{A}} = \frac{1}{n} \cdot \bar{\mathbf{S}}^\top \bar{\mathbf{S}}$ be the covariance matrix of the sketched data. Then, instead of \mathbf{A} , we can approximately solve the sparse PCA problem by applying Algorithm 1 on the low-rank surrogate $\bar{\mathbf{A}}$. The above are formally outlined in Algorithm 3. We note that the covariance matrix $\bar{\mathbf{A}}$ does not need to be explicitly computed; Algorithm 1 can operate directly on the (sketched) input data matrix.

Algorithm 3 Sparse PCA on Low Dim. Sketch

input : Real $n \times d$ \mathbf{S} , $r \in \mathbb{Z}_+$, $\epsilon \in (0, 1)$, $k \in \mathbb{Z}_+$.

output $\bar{\mathbf{X}}_{(r)} \in \mathcal{X}_k$. {Thm. 2}

1: $\bar{\mathbf{S}} \leftarrow \text{SKETCH}(\mathbf{S}, r)$

2: $\bar{\mathbf{A}} \leftarrow \bar{\mathbf{S}}^\top \bar{\mathbf{S}}$

3: $\bar{\mathbf{X}}_{(r)} \leftarrow \text{ALGORITHM 1}(\bar{\mathbf{A}}, \epsilon, k)$.

Theorem 2. For any $n \times d$ input data matrix \mathbf{S} , with corresponding empirical covariance matrix $\mathbf{A} = 1/n \cdot \mathbf{S}^\top \mathbf{S}$, any desired number of components k , and accuracy parameters $\epsilon \in (0, 1)$ and r , Algorithm 3 outputs $\mathbf{X}_{(r)} \in \mathcal{X}_k$ such that

$$\text{Tr}(\mathbf{X}_{(r)}^\top \mathbf{A} \mathbf{X}_{(r)}) \geq (1 - \epsilon) \cdot \text{Tr}(\mathbf{X}_\star^\top \mathbf{A} \mathbf{X}_\star) - 2 \cdot k \cdot \lambda_{1,s}(\mathbf{A} - \bar{\mathbf{A}}),$$

in time $T_{\text{SKETCH}}(r) + T_{\text{SVD}}(r) + O\left(\left(\frac{4}{\epsilon}\right)^{r \cdot k} \cdot d \cdot (s \cdot k)^2\right)$. Here, $\mathbf{X}_\star \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}_k} \text{Tr}(\mathbf{X}^\top \mathbf{A} \mathbf{X})$, and $\lambda_{1,s}(\mathbf{A})$ denotes the sparse eigenvalue, i.e., the eigenvalue that corresponds to the principal s -sparse eigenvector of \mathbf{A} .

The error $\lambda_{1,s}(\mathbf{A} - \bar{\mathbf{A}})$ and in turn the tightness of the approximation guarantees hinges on the quality of the sketch $\bar{\mathbf{A}}$. Higher values of the parameter r (the rank of the sketch) can allow for a more accurate solution and tighter guarantees. That is the case, for example, when the sketch is obtained through exact SVD. In that sense, Theorem 2 establishes a natural trade-off between the running time of Algorithm 3 and the quality of the approximation guarantees. A formal proof of Theorem 2 is provided in Section 9.3. Observe that the error term itself is a sparse eigenvalue that is hard to approximate, however even loose bounds provide tight conditional approximation results, as we see next.

Using the main matrix approximation result of [31], the next theorem establishes that Algorithm 3 can be turned into an additive PTAS.

Theorem 3. Let \mathbf{A} be a $d \times d$ positive semidefinite matrix with entries in $[-1, 1]$, \mathbf{V} be a $d \times d$ matrix such that $\mathbf{A} = \mathbf{V} \mathbf{V}^\top$. Further, let \mathbf{R} be a random $d \times r$ matrix with entries drawn i.i.d. according to $\mathcal{N}(0, 1/r)$, and define

$$\bar{\mathbf{A}} \triangleq \mathbf{V} \mathbf{R} \mathbf{R}^\top \mathbf{V}^\top.$$

For any constant $\epsilon \in (0, 1]$, let $r = O(\epsilon^{-2} \log d)$. Then, for any desired sparsity s , and number of components $k = O(1)$, Algorithm 1 with input argument $\bar{\mathbf{A}}$ and accuracy parameter ϵ , outputs $\mathbf{X}_{(r)} \in \mathcal{X}_k$ such that

$$\text{Tr}(\mathbf{X}_{(r)}^\top \mathbf{A} \mathbf{X}_{(r)}) \geq \text{Tr}(\mathbf{X}_\star^\top \mathbf{A} \mathbf{X}_\star) - \epsilon \cdot s$$

with probability at least $1 - 1/\text{poly}(d)$, in time $n^{O(\log(1/\epsilon)/\epsilon^2)}$.

Remark 3.1. Note that $\lambda_1(\mathbf{A} - \bar{\mathbf{A}})$ serves as another elementary upper bound on $\lambda_{1,s}(\mathbf{A} - \bar{\mathbf{A}})$. If $\bar{\mathbf{A}}$ is a the rank- d SVD approximation of \mathbf{A} , then—similar to [32]—we can obtain a multiplicative PTAS for sparse PCA, under the assumption of a decaying spectrum (e.g., under a power-law decay), and for $s = \Omega(n)$.

4 Related Work

We are not aware of any algorithm with provable guarantees for sparse PCA with *disjoint supports*. Multiple components can be extracted by repeatedly solving (1) using one of the aforementioned methods. To ensure disjoint supports, variables “selected” by a component are removed from the dataset. This greedy approach, however, can result in highly suboptimal objective value (See example in Sec. 7).

A significant volume of work has focused on the single-component sparse PCA problem (1); we scratch the surface and refer the reader to citations therein. Representative examples range from early heuristics in [2], to the LASSO based techniques in [3], the elastic net ℓ_1 -regression in [4], ℓ_1 and ℓ_0 regularized optimization methods such as GPower in [7], a greedy branch-and-bound

technique in [8], or semidefinite programming approaches [9, 10, 11]. The authors of [13] present an approach that uses ideas from an expectation-maximization (EM) formulation of the problem. More recently, [12] presents a simple and very efficient truncated version of the power iteration (TPower). Finally, [15] introduces an exact solver for the low-rank case of the problem; this solver was then used on low-rank sketches in the work of [14] (SpanSPCA), that provides conditional approximation guarantees under spectral assumptions on the input data. Several ideas in this work are inspired by the aforementioned low-rank solvers. In our experiments, we compare against EM, TPower, and SpanSPCA, which all are experimentally achieving state-of-the-art performance.

Parallel to the algorithmic and optimization perspective, there is large line of statistical analysis for sparse PCA that focuses on guarantees pertaining to planted models and the recovery of a “true” sparse component [16, 17, 18, 19, 20, 21, 22, 23, 24].

There has been some work on the explicit estimation of principal subspaces or multiple components under sparsity constraints. Non-deflation-based algorithms include extensions of the diagonal thresholding algorithm [33] and iterative thresholding approaches [17], while [34] and [35] propose methods that rely on the “row sparsity for subspaces” assumption of [26]. These methods yield components supported on a common set of variables, and hence solve a problem different from (2). Magdon-Ismail and Boutsidis [27] discuss the multiple component Sparse PCA problem, propose an alternative objective function and for that problem obtain interesting theoretical guarantees. Finally, [36] develops a framework for sparse matrix factorization problems, based on a novel atomic norm. That framework captures sparse PCA – although not explicitly the constraint of disjoint supports – but the resulting optimization problem, albeit convex, is NP-hard.

5 Experiments

We evaluate our algorithm on a series of real datasets, and compare it to deflation-based approaches for sparse PCA using TPower [12], EM [13], and SpanSPCA [14]. The latter are representative of the state of the art for the single-component sparse PCA problem (1). Multiple components are computed one by one. To ensure disjoint supports, the deflation step effectively amounts to removing from the dataset all variables used by previously extracted components. For algorithms that are randomly initialized, we depict best results over multiple random restarts. Additional experimental results are listed in Section 11 of the appendix.

Our experiments are conducted in a Matlab environment. Due to its nature, our algorithm is easily parallelizable; its prototypical implementation utilizes the Parallel Pool Matlab feature to exploit multicore (or distributed cluster) capabilities. Recall that our algorithm operates on a low-rank approximation of the input data. Unless otherwise specified, it is configured for a rank-4 approximation obtained via truncated SVD. Finally, we put a time barrier in the execution of our algorithm, at the cost of the theoretical approximation guarantees; the algorithm returns best results at the time of termination. This “early termination” can only hurt the performance of our algorithm.

Leukemia Dataset. We evaluate our algorithm on the Leukemia dataset [37]. The dataset comprises 72 samples, each consisting of expression values for 12582 probe sets. We extract $k = 5$ sparse components, each active on $s = 50$ features. In Fig. 2(a), we plot the cumulative explained variance versus the number of components. Deflation-based approaches are greedy: the leading components capture high values of variance, but subsequent ones contribute less. On the contrary, our algorithm jointly optimizes the $k = 5$ components and achieves higher *total* cumulative variance; one cannot identify a top component. We repeat the experiment for multiple values of k . Fig. 2(b) depicts the total cumulative variance capture by each method, for each value of k .

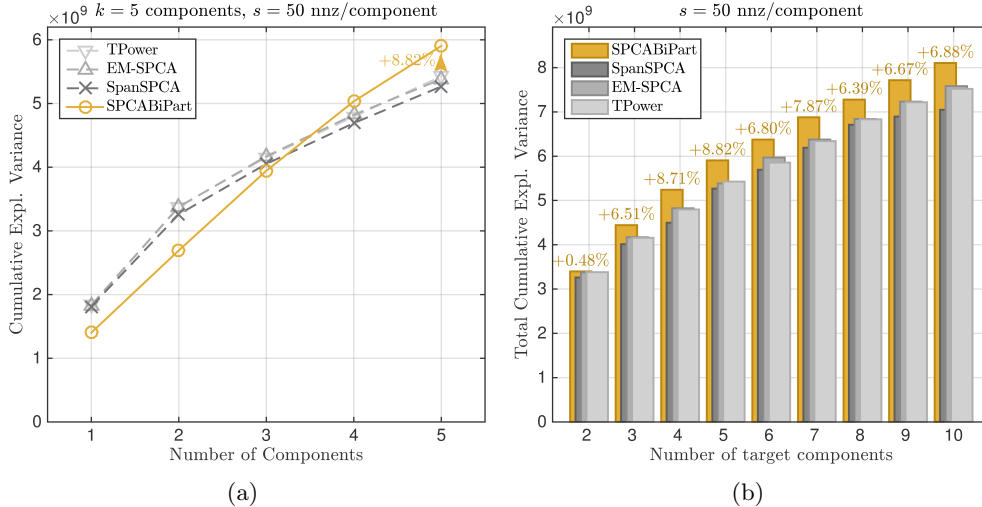


Figure 2: Cumulative variance captured by the k s -sparse extracted components – Leukemia dataset [37]. Sparsity is arbitrarily set to $s = 50$ nonzero entries per component. Fig. 2(a) depicts the cum. variance versus the number of components, for $k = 5$. Deflation-based approaches are greedy; first components capture high variance, but subsequent ones contribute less. Our algorithm jointly optimizes the $k = 5$ components and achieves higher *total* cum. variance. Fig. 2(b) depicts the total cum. variance achieved for various values of k .

Additional Datasets. We repeat the experiment on multiple datasets, arbitrarily selected from [37]. Table 1 lists the total cumulative variance captured by $k = 5$ components, each with $s = 40$ nonzero entries, extracted using the four methods. Our algorithm achieves the highest values in most cases.

Bag of Words (BoW) Dataset. [37] This is a collection of text corpora stored under the “bag-of-words” model. For each text corpus, a vocabulary of d words is extracted upon tokenization, and the removal of stopwords and words appearing fewer than ten times in total. Each document is then represented as a vector in that d -dimensional space, with the i th entry corresponding to the number of appearances of the i th vocabulary entry in the document.

We solve the sparse PCA problem (2) on the word-by-word cooccurrence matrix, and extract $k = 8$ sparse components, each with cardinality $s = 10$. We note that the latter is not explicitly constructed; our algorithm can operate directly on the input word-by-document matrix. Table 2 lists the variance captured by each method; our algorithm consistently outperforms the other

		TPower	EM sPCA	SpanSPCA	SPCABiPart
AMZN COM REV	(1500×10000)	7.31e + 03	7.32e + 03	7.31e + 03	7.79e + 03
ARCENCE TRAIN	(100×10000)	1.08e + 07	1.02e + 07	1.08e + 07	1.10e + 07
CBCL FACE TRAIN	(2429×361)	5.06e + 00	5.18e + 00	5.23e + 00	5.29e + 00
ISOLET-5	(1559×617)	3.31e + 01	3.43e + 01	3.34e + 01	3.51e + 01
LEUKEMIA	(72×12582)	5.00e + 09	5.03e + 09	4.84e + 09	5.37e + 09
PEMS TRAIN	(267×138672)	3.94e + 00	3.58e + 00	3.89e + 00	3.75e + 00
MFEAT PIX	(2000×240)	5.00e + 02	5.27e + 02	5.08e + 02	5.47e + 02

Table 1: Total cumulative variance captured by $k = 5$ 40-sparse extracted components on various datasets [37]. For each dataset, we list the size ($\#$ samples $\times\#$ variables) and the value of variance captured by each method. Our algorithm operates on a rank-4 sketch in all cases.

		TPower	EM sPCA	SpanSPCA	SPCABiPart
BoW:NIPS	(1500×12419)	2.51e + 03	2.57e + 03	2.53e + 03	3.34e + 03 (+29.98%)
BoW:KOS	(3430×6906)	4.14e + 01	4.24e + 01	4.21e + 01	6.14e + 01 (+44.57%)
BoW:ENRON	(39861×28102)	2.11e + 02	2.00e + 02	2.09e + 02	2.38e + 02 (+12.90%)
BoW:NYTIMES	(300000×102660)	4.81e + 01	–	4.81e + 01	5.31e + 01 (+10.38%)

Table 2: Total variance captured by $k = 8$ extracted components, each with $s = 15$ nonzero entries – Bag of Words dataset [37]. For each corpus, we list the size ($\#documents \times \#vocabulary-size$) and the explained variance. Our algorithm operates on a rank-5 sketch in all cases.

approaches.

Finally, note that here each sparse component effectively *selects* a small set of words. In turn, the k extracted components can be interpreted as a set of well-separated *topics*. In Table 3, we list the topics extracted from the NY Times corpus (part of the Bag of Words dataset). The corpus consists of $3 \cdot 10^5$ news articles and a vocabulary of $d = 102660$ words.

	Topic 1	Topic 2	Topic 3	Topic 4	Topic 5	Topic 6	Topic 7	Topic 8
1:	percent	zzz_united_states	zzz_bush	company	team	cup	school	zzz_al_gore
2:	million	zzz_u_s	official	companies	game	minutes	student	zzz_george_bush
3:	money	zzz_american	government	market	season	add	children	campaign
4:	high	attack	president	stock	player	tablespoon	women	election
5:	program	military	group	business	play	oil	show	plan
6:	number	palestinian	leader	billion	point	teaspoon	book	tax
7:	need	war	country	analyst	run	water	family	public
8:	part	administration	political	firm	right	pepper	look	zzz_washington
9:	problem	zzz_white_house	american	sales	home	large	hour	member
10:	com	games	law	cost	won	food	small	nation

Table 3: BoW:NYTIMES dataset [37]. The table lists the words corresponding to the $s = 10$ nonzero entries of each of the $k = 8$ extracted components (topics). Words corresponding to higher magnitude entries appear higher in the topic.

6 Conclusions

We considered the sparse PCA problem for multiple components with disjoint supports. Existing methods for the single component problem can be used along with an appropriate deflation step to compute multiple components one by one, leading to potentially suboptimal results. We presented a novel algorithm for jointly optimizing multiple sparse and disjoint components with provable approximation guarantees. Our algorithm is combinatorial and exploits interesting connections between the sparse PCA and the bipartite maximum weight matching problems. It runs in time that grows as a low-order polynomial in the ambient dimension of the input data, but depends exponentially on its rank. To alleviate this dependency, we can apply the algorithm on a low-dimensional sketch of the input, at the cost of an additional error in our theoretical approximation guarantees. Empirical evaluation of our algorithm demonstrated that in many cases it outperforms deflation-based approaches.

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References

- [1] H.F. Kaiser. The varimax criterion for analytic rotation in factor analysis. *Psychometrika*, 23(3):187–200, 1958.
- [2] I.T. Jolliffe. Rotation of principal components: choice of normalization constraints. *Journal of Applied Statistics*, 22(1):29–35, 1995.
- [3] I.T. Jolliffe, N.T. Trendafilov, and M. Uddin. A modified principal component technique based on the lasso. *Journal of Computational and Graphical Statistics*, 12(3):531–547, 2003.
- [4] Hui Zou, Trevor Hastie, and Robert Tibshirani. Sparse principal component analysis. *Journal of computational and graphical statistics*, 15(2):265–286, 2006.
- [5] Christos Boutsidis, Petros Drineas, and Malik Magdon-Ismael. Sparse features for pca-like linear regression. In *Advances in Neural Information Processing Systems*, pages 2285–2293, 2011.
- [6] Siu On Chan, Dimitris Papailiopoulos, and Aviad Rubinstein. On the worst-case approximability of sparse PCA. *preprint*, 2015.
- [7] M. Journée, Y. Nesterov, P. Richtárik, and R. Sepulchre. Generalized power method for sparse principal component analysis. *The Journal of Machine Learning Research*, 11:517–553, 2010.
- [8] B. Moghaddam, Y. Weiss, and S. Avidan. Spectral bounds for sparse pca: Exact and greedy algorithms. *NIPS*, 18:915, 2006.
- [9] Alexandre d’Aspremont, Francis Bach, and Laurent El Ghaoui. Optimal solutions for sparse principal component analysis. *The Journal of Machine Learning Research*, 9:1269–1294, 2008.
- [10] Y. Zhang, A. d’Aspremont, and L.E. Ghaoui. Sparse pca: Convex relaxations, algorithms and applications. *Handbook on Semidefinite, Conic and Polynomial Optimization*, pages 915–940, 2012.
- [11] A. d’Aspremont, L. El Ghaoui, M.I. Jordan, and G.R.G. Lanckriet. A direct formulation for sparse pca using semidefinite programming. *SIAM review*, 49(3):434–448, 2007.
- [12] Xiao-Tong Yuan and Tong Zhang. Truncated power method for sparse eigenvalue problems. *The Journal of Machine Learning Research*, 14(1):899–925, 2013.
- [13] Christian D. Sigg and Joachim M. Buhmann. Expectation-maximization for sparse and non-negative pca. In *Proceedings of the 25th International Conference on Machine Learning, ICML ’08*, pages 960–967, New York, NY, USA, 2008. ACM.
- [14] Dimitris Papailiopoulos, Alexandros Dimakis, and Stavros Korokythakis. Sparse pca through low-rank approximations. In *Proceedings of The 30th International Conference on Machine Learning*, pages 747–755, 2013.

- [15] Megasthenis Asteris, Dimitris S. Papailiopoulos, and Georgios N. Karystinos. The sparse principal component of a constant-rank matrix. *Information Theory, IEEE Transactions on*, 60(4):2281–2290, April 2014.
- [16] Arash Amini and Martin Wainwright. High-dimensional analysis of semidefinite relaxations for sparse principal components. In *Information Theory, 2008. ISIT 2008. IEEE International Symposium on*, pages 2454–2458. IEEE, 2008.
- [17] Zongming Ma. Sparse principal component analysis and iterative thresholding. *The Annals of Statistics*, 41(2):772–801, 2013.
- [18] A. d’Aspremont, F. Bach, and L.E. Ghaoui. Approximation bounds for sparse principal component analysis. *arXiv preprint arXiv:1205.0121*, 2012.
- [19] T Tony Cai, Zongming Ma, and Yihong Wu. Sparse pca: Optimal rates and adaptive estimation. *arXiv preprint arXiv:1211.1309*, 2012.
- [20] Yash Deshpande and Andrea Montanari. Sparse pca via covariance thresholding. *arXiv preprint arXiv:1311.5179*, 2013.
- [21] Quentin Berthet and Philippe Rigollet. Optimal detection of sparse principal components in high dimension. *Ann. Statist.*, 41(1):1780–1815, 2013.
- [22] Q. Berthet and P. Rigollet. Complexity theoretic lower bounds for sparse principal component detection. *Journal of Machine Learning Research (JMLR)*, 30:1046–1066 (electronic), 2013.
- [23] Tengyao Wang, Quentin Berthet, and Richard J. Samworth. Statistical and computational trade-offs in estimation of sparse principal components. *arXiv preprint arXiv:1408.5369*, 2014.
- [24] Robert Krauthgamer, Boaz Nadler, and Dan Vilenchik. Do semidefinite relaxations solve sparse PCA up to the information limit? *Annals of Probability*, 43:1300–1322, 2015.
- [25] L. Mackey. Deflation methods for sparse pca. *NIPS*, 21:1017–1024, 2009.
- [26] Vincent Vu and Jing Lei. Minimax rates of estimation for sparse pca in high dimensions. In *International Conference on Artificial Intelligence and Statistics*, pages 1278–1286, 2012.
- [27] Malik Magdon-Ismail and Christos Boutsidis. Optimal sparse linear auto-encoders and sparse PCA. *CoRR*, abs/1502.06626, 2015.
- [28] Jiří Matoušek. *Lectures on discrete geometry*, volume 212. Springer New York, 2002.
- [29] Lyle Ramshaw and Robert E Tarjan. On minimum-cost assignments in unbalanced bipartite graphs. *HP Labs, Palo Alto, CA, USA, Tech. Rep. HPL-2012-40R1*, 2012.
- [30] Nathan Halko, Per-Gunnar Martinsson, and Joel A Tropp. Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions. *SIAM review*, 53(2):217–288, 2011.
- [31] Noga Alon, Troy Lee, Adi Shraibman, and Santosh Vempala. The approximate rank of a matrix and its algorithmic applications: approximate rank. In *Proceedings of the forty-fifth annual ACM symposium on Theory of computing*, pages 675–684. ACM, 2013.

- [32] Megasthenis Asteris, Dimitris Papailiopoulos, and Alexandros Dimakis. Nonnegative sparse pca with provable guarantees. In *Proceedings of the 31st International Conference on Machine Learning (ICML-14)*, pages 1728–1736, 2014.
- [33] Iain M Johnstone and Arthur Yu Lu. On consistency and sparsity for principal components analysis in high dimensions. *Journal of the American Statistical Association*, 104(486), 2009.
- [34] Vincent Q Vu, Juhee Cho, Jing Lei, and Karl Rohe. Fantope projection and selection: A near-optimal convex relaxation of sparse pca. In *NIPS*, pages 2670–2678, 2013.
- [35] Zhaoran Wang, Huanran Lu, and Han Liu. Nonconvex statistical optimization: minimax-optimal sparse pca in polynomial time. *arXiv preprint arXiv:1408.5352*, 2014.
- [36] Emile Richard, Guillaume R Obozinski, and Jean-Philippe Vert. Tight convex relaxations for sparse matrix factorization. In *Advances in Neural Information Processing Systems*, pages 3284–3292, 2014.
- [37] M. Lichman. UCI machine learning repository, 2013.
- [38] Sanjoy Dasgupta and Anupam Gupta. An elementary proof of a theorem of johnson and lindenstrauss. *Random structures and algorithms*, 22(1):60–65, 2003.

Supplemental Material

7 On the sub-optimality of deflation – An example

We provide a simple example demonstrating the sub-optimality of deflation based approaches for computing multiple sparse components with disjoint supports. Consider the real 4×4 matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & \epsilon \\ 0 & \delta & 0 & 0 \\ 0 & 0 & \delta & 0 \\ \epsilon & 0 & 0 & 1 \end{bmatrix},$$

with $\epsilon, \delta > 0$ such that $\epsilon + \delta < 1$. Note that \mathbf{A} is PSD; $\mathbf{A} = \mathbf{B}^\top \mathbf{B}$ for

$$\mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & \epsilon \\ 0 & \sqrt{\delta} & 0 & 0 \\ 0 & 0 & \sqrt{\delta} & 0 \\ 0 & 0 & 0 & \sqrt{1 - \epsilon^2} \end{bmatrix}.$$

We seek two 2-sparse components with disjoint supports, *i.e.*, the solution to

$$\max_{\mathbf{X} \in \mathcal{X}} \sum_{j=1}^2 \mathbf{x}_j^\top \mathbf{A} \mathbf{x}_j, \tag{8}$$

where

$$\mathcal{X} \triangleq \{ \mathbf{X} \in \mathbb{R}^{4 \times 2} : \|\mathbf{x}_i\|_2 \leq 1, \|\mathbf{x}_i\|_0 \leq 2 \forall i \in \{1, 2\}, \text{supp}(\mathbf{x}_1) \cap \text{supp}(\mathbf{x}_2) = \emptyset \}.$$

Iterative computation with deflation. Following an iterative, greedy procedure with a deflation step, we compute one component at the time. The first component is

$$\mathbf{x}_1 = \arg \max_{\|\mathbf{x}\|_0=2, \|\mathbf{x}\|_2=1} \mathbf{x}^\top \mathbf{A} \mathbf{x}. \quad (9)$$

Recall that for any unit norm vector \mathbf{x} with support $I = \text{supp}(\mathbf{x})$,

$$\mathbf{x}^\top \mathbf{A} \mathbf{x} \leq \lambda_{\max}(\mathbf{A}_{I,I}), \quad (10)$$

where $\mathbf{A}_{I,I}$ denotes the principal submatrix of \mathbf{A} formed by the rows and columns indexed by I . Equality can be achieved in (10) for \mathbf{x} equal to the leading eigenvector of $\mathbf{A}_{I,I}$. Hence, it suffices to determine the optimal support for \mathbf{x}_1 . Due to the small size of the example, it is easy to determine that the set $I_1 = \{1, 4\}$ maximizes the objective in (10) over all sets of two indices, achieving value

$$\mathbf{x}_1^\top \mathbf{A} \mathbf{x}_1 = \lambda_{\max} \left(\begin{bmatrix} 1 & \epsilon \\ \epsilon & 1 \end{bmatrix} \right) = 1 + \epsilon. \quad (11)$$

Since subsequent components must have disjoint supports, it follows that the support of the second 2-sparse component \mathbf{x}_2 is $I_2 = \{2, 3\}$, and \mathbf{x}_2 achieves value

$$\mathbf{x}_2^\top \mathbf{A} \mathbf{x}_2 = \lambda_{\max} \left(\begin{bmatrix} \delta & 0 \\ 0 & \delta \end{bmatrix} \right) = \delta. \quad (12)$$

In total, the objective value in (8) achieved by the greedy computation with a deflation step is

$$\sum_{j=1}^2 \mathbf{x}_j^\top \mathbf{A} \mathbf{x}_j = 1 + \epsilon + \delta. \quad (13)$$

The sub-optimality of deflation. Consider an alternative pair of 2-sparse components \mathbf{x}'_1 and \mathbf{x}'_2 with support sets $I'_1 = \{1, 2\}$ and $I'_2 = \{3, 4\}$, respectively. Based on the above, such a pair achieves objective value in (8) equal to

$$\lambda_{\max} \left(\begin{bmatrix} 1 & 0 \\ 0 & \delta \end{bmatrix} \right) + \lambda_{\max} \left(\begin{bmatrix} \delta & 0 \\ 0 & 1 \end{bmatrix} \right) = 1 + 1 = 2,$$

which clearly outperforms the objective value in (13) (under the assumption $\epsilon + \delta < 1$), demonstrating the sub-optimality of the $\mathbf{x}_1, \mathbf{x}_2$ pair computed by the deflation-based approach. In fact, for small ϵ, δ the objective value in the second case is larger than the former by almost a factor of two.

8 Construction of Bipartite Graph

The following algorithm formally outlines the steps for generating the bipartite graph $G = (\{U_j\}_{j=1}^k, V, E)$ given a *weight* $d \times k$ matrix \mathbf{W} .

Algorithm 4 Generate Bipartite Graph

input Real $d \times k$ matrix \mathbf{W}
output Bipartite $G = (\{U_j\}_{j=1}^k, V, E)$

{Fig. 1}

 1: **for** $j = 1, \dots, k$ **do**

 2: $U_j \leftarrow \{u_1^{(j)}, \dots, u_s^{(j)}\}$

 3: **end for**

 4: $U \leftarrow \cup_{j=1}^k U_j$
 $\{|U| = k \cdot s\}$

 5: $V \leftarrow \{1, \dots, d\}$

 6: $E \leftarrow U \times V$

 7: **for** $i = 1, \dots, d$ **do**

 8: **for** $j = 1, \dots, k$ **do**

 9: **for each** $u \in U_j$ **do**

 10: $w(u, v_i) \leftarrow W_{ij}^2$

 11: **end for**

 12: **end for**

 13: **end for**

9 Proofs

9.1 Guarantees of Algorithm 2

Lemma 2.1. For any real $d \times k$ matrix \mathbf{W} , and Algorithm 2 outputs

$$\tilde{\mathbf{X}} = \arg \max_{\mathbf{X} \in \mathcal{X}_k} \sum_{j=1}^k \langle \mathbf{X}^j, \mathbf{W}^j \rangle^2 \quad (14)$$

in time $O(d \cdot (s \cdot k)^2)$.

Proof. Consider a matrix $\mathbf{X} \in \mathcal{X}_k$ and let I_j , $j = 1, \dots, k$ denote the support sets of its columns. By the constraints in \mathcal{X}_k , those sets are disjoint, *i.e.*, $I_{j_1} \cap I_{j_2} = \emptyset \forall j_1, j_2 \in \{1, \dots, k\}, j_1 \neq j_2$, and

$$\sum_{j=1}^k \langle \mathbf{X}^j, \mathbf{W}^j \rangle^2 = \sum_{j=1}^k \left(\sum_{i \in I_j} X_{ij} \cdot W_{ij} \right)^2 \leq \sum_{j=1}^k \left(\sum_{i \in I_j} W_{ij}^2 \right). \quad (15)$$

The last inequality is due to Cauchy-Schwarz and the fact that $\|\mathbf{X}^j\|_2 \leq 1, \forall j \in \{1, \dots, k\}$. In fact, if the supports sets I_j , $j = 1, \dots, k$ were known, the upper bound in (15) would be achieved by setting $\mathbf{X}_{I_j}^j = \mathbf{W}_{I_j}^j / \|\mathbf{W}_{I_j}^j\|_2$, *i.e.*, setting the nonzero subvector of the j th column of \mathbf{X} colinear to the corresponding subvector of the j th column of \mathbf{W} . Hence, the key step towards computing the optimal solution $\tilde{\mathbf{X}}$ is to determine the support sets I_j , $j = 1, \dots, k$ of its columns.

Consider the set of binary matrices

$$\mathcal{Z} \triangleq \left\{ \mathbf{Z} \in \{0, 1\}^{d \times k} : \|\mathbf{Z}^j\|_0 \leq s \forall j \in [k], \text{supp}(\mathbf{Z}^i) \cap \text{supp}(\mathbf{Z}^j) = \emptyset \forall i, j \in [k], i \neq j \right\}.$$

The set represents all possible supports for the members of \mathcal{X}_k . Taking into account the previous discussion, the maximization in (14) can be written with respect to $\mathbf{Z} \in \mathcal{Z}$:

$$\max_{\mathbf{X} \in \mathcal{X}_k} \sum_{j=1}^k \langle \mathbf{X}^j, \mathbf{W}^j \rangle^2 = \max_{\mathbf{Z} \in \mathcal{Z}} \sum_{j=1}^k \sum_{i=1}^d Z_{ij} W_{ij}^2. \quad (16)$$

Let $\tilde{\mathbf{Z}} \in \mathcal{Z}$ denote the optimal solution, which corresponds to the (support) indicator of $\tilde{\mathbf{X}}$. Next, we show that computing $\tilde{\mathbf{Z}}$ boils down to solving a maximum weight matching problem on the bipartite graph generated by Algorithm 4. Recall that given $\mathbf{W} \in \mathbb{R}^{d \times k}$, Algorithm 4 generates a complete weighted bipartite graph $G = (U, V, E)$ where

- V is a set of d vertices v_1, \dots, v_d , corresponding to the d variables, *i.e.*, the d rows of $\hat{\mathbf{X}}$.
- U is a set of $k \cdot s$ vertices, conceptually partitioned into k disjoint subsets U_1, \dots, U_k , each of cardinality s . The j th subset, U_j , is associated with the support \mathcal{I}_j ; the s vertices $u_\alpha^{(j)}$, $\alpha = 1, \dots, s$ in U_j serve as placeholders for the variables/indices in \mathcal{I}_j .
- Finally, the edge set is $E = U \times V$. The edge weights are determined by the $d \times k$ matrix \mathbf{W} in (6). In particular, the weight of edge $(u_\alpha^{(j)}, v_i)$ is equal to W_{ij}^2 . Note that all vertices in U_j are effectively identical; they all share a common neighborhood and edge weights.

It is straightforward to verify that any $\mathbf{Z} \in \mathcal{Z}$ corresponds to a perfect matching in G and vice versa; $Z_{ij} = 1$ if and only if vertex $v_i \in V$ is matched with a vertex in U_j (all vertices in U_j are equivalent with respect to their neighborhood). Further, the objective value in (16) for a given $\mathbf{Z} \in \mathcal{Z}$ is equal to the weight of the corresponding matching in G . More formally,

- Given a perfect matching \mathcal{M} , the support I_j of the j th column of \mathbf{Z} is determined by the neighborhood of U_j in the matching:

$$I_j \leftarrow \{i \in [d] : (u, v_i) \in \mathcal{M}, u \in U_j\}, \quad j = 1, \dots, k. \quad (17)$$

Note that the sets I_j , $j = 1, \dots, k$ are indeed disjoint, and each has cardinality equal to s . The weight of the matching \mathcal{M} is

$$\sum_{(u,v) \in \mathcal{M}} w(u,v) = \sum_{j=1}^k \sum_{\substack{(u,v_i) \in \mathcal{M}: \\ u \in U_j}} w(u,v_i) = \sum_{j=1}^k \sum_{i \in I_j} W_{ij}^2 = \sum_{j=1}^k \sum_{i=1}^d Z_{ij} \cdot W_{ij}^2, \quad (18)$$

which is equal to the objective function in (16).

- Conversely, given an indicator matrix $\mathbf{Z} \in \mathcal{Z}$, let $I_j \triangleq \text{supp}(\mathbf{Z}^j)$, and let $I_j(\alpha)$ denote the α th element in the set, $\alpha = 1, \dots, s$ (with an arbitrary ordering). Then,

$$\mathcal{M} = \left\{ (u_\alpha^{(j)}, v_{I_j(\alpha)}), \alpha = 1, \dots, s, j = 1, \dots, k \right\} \subset E$$

is a perfect matching in G . The objective value achieved by \mathbf{Z} is equal to the weight of \mathcal{M} :

$$\sum_{j=1}^k \sum_{i=1}^d Z_{ij} \cdot W_{ij}^2 = \sum_{j=1}^k \sum_{i \in I_j} W_{ij}^2 = \sum_{j=1}^k \sum_{\alpha=1}^s W_{I_j(\alpha),j}^2 = \sum_{(u,v) \in \mathcal{M}} w(u,v). \quad (19)$$

It follows from (18) and (19) that to determine $\tilde{\mathbf{Z}}$, it suffices to compute a maximum weight perfect matching in G . The desired support is then obtained as described in (17) (lines 4-7 of Algorithm 2). This complete the proof of correctness of Algorithm 2 which proceeds in the steps described above to determine the support of $\tilde{\mathbf{X}}$.

The weighted bipartite graph G is generated in $O(d \cdot (s \cdot k))$. The running time of Algorithm 2 is dominated by computing the maximum weight matching of G . For the case of unbalanced bipartite graph with $|U| = s \cdot k < d = |V|$ the Hungarian algorithm can be modified [29] to compute the maximum weight bipartite matching in time $O(|E||U| + |U|^2 \log |U|) = O(d \cdot (s \cdot k)^2)$. This completes the proof. \square

9.2 Guarantees of Algorithm 1 – Proof of Theorem 1

We first prove a more general version of Theorem 1 for arbitrary constraint sets. Combining that with the guarantees of Algorithm 2, we prove the Theorem 1.

Lemma 9.2. *For any real $d \times d$ rank- r PSD matrix $\bar{\mathbf{A}}$ and arbitrary set $\mathcal{X} \subset \mathbb{R}^{d \times k}$, let $\bar{\mathbf{X}}_\star \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}} \text{Tr}(\mathbf{X}^\top \bar{\mathbf{A}} \mathbf{X})$. Assuming that there exists an operator $P_{\mathcal{X}} : \mathbb{R}^{d \times k} \rightarrow \mathcal{X}$ such that $P_{\mathcal{X}}(\mathbf{W}) \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}} \langle \mathbf{x}_j, \mathbf{w}_j \rangle^2$, then Algorithm 1 outputs $\bar{\mathbf{X}} \in \mathcal{X}$ such that*

$$\text{Tr}(\bar{\mathbf{X}}^\top \bar{\mathbf{A}} \bar{\mathbf{X}}) \geq (1 - \epsilon) \cdot \text{Tr}(\bar{\mathbf{X}}_\star^\top \bar{\mathbf{A}} \bar{\mathbf{X}}_\star),$$

in time $T_{\text{SVD}}(r) + O\left(\left(\frac{4}{\epsilon}\right)^{r \cdot k} \cdot (T_{\mathcal{X}} + kd)\right)$, where $T_{\mathcal{X}}$ is the time required to compute $P_{\mathcal{X}}(\cdot)$ and $T_{\text{SVD}}(r)$ the time required to compute the truncated SVD of $\bar{\mathbf{A}}$.

Proof. Let $\bar{\mathbf{A}} = \bar{\mathbf{U}} \bar{\mathbf{\Lambda}} \bar{\mathbf{U}}^\top$ denote the truncated eigenvalue decomposition of $\bar{\mathbf{A}}$; $\bar{\mathbf{\Lambda}}$ is a diagonal $r \times r$ whose i th diagonal entry Λ_{ii} is equal to the i th largest eigenvalue of $\bar{\mathbf{A}}$, while the columns of $\bar{\mathbf{U}}$ contain the corresponding eigenvectors. By the Cauchy-Schwartz inequality, for any $\mathbf{x} \in \mathbb{R}^d$,

$$\mathbf{x}^\top \bar{\mathbf{A}} \mathbf{x} = \|\bar{\mathbf{\Lambda}}^{1/2} \bar{\mathbf{U}}^\top \mathbf{x}\|_2^2 \geq \langle \bar{\mathbf{\Lambda}}^{1/2} \bar{\mathbf{U}}^\top \mathbf{x}, \mathbf{c} \rangle^2, \quad \forall \mathbf{c} \in \mathbb{R}^r : \|\mathbf{c}\|_2 = 1. \quad (20)$$

In fact, equality in (20) is achieved for \mathbf{c} colinear to $\bar{\mathbf{\Lambda}}^{1/2} \bar{\mathbf{U}}^\top \mathbf{x}$, and hence,

$$\mathbf{x}^\top \bar{\mathbf{A}} \mathbf{x} = \max_{\mathbf{c} \in \mathbb{S}_2^{r-1}} \langle \bar{\mathbf{\Lambda}}^{1/2} \bar{\mathbf{U}}^\top \mathbf{x}, \mathbf{c} \rangle^2. \quad (21)$$

In turn,

$$\text{Tr}(\mathbf{X}^\top \bar{\mathbf{A}} \mathbf{X}) = \sum_{j=1}^k \mathbf{X}^j \top \bar{\mathbf{A}} \mathbf{X}^j = \max_{\mathbf{C} : \mathbf{C}^j \in \mathbb{S}_2^{r-1} \forall j} \sum_{j=1}^k \langle \bar{\mathbf{\Lambda}}^{1/2} \bar{\mathbf{U}}^\top \mathbf{X}^j, \mathbf{C}^j \rangle^2. \quad (22)$$

Recall that $\bar{\mathbf{X}}_\star$ is the optimal solution of the trace maximization on $\bar{\mathbf{A}}$, *i.e.*,

$$\bar{\mathbf{X}}_\star \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}} \text{Tr}(\mathbf{X}^\top \bar{\mathbf{A}} \mathbf{X}).$$

Let $\bar{\mathbf{C}}_\star$ be the maximizing value of \mathbf{C} in (22) for $\mathbf{X} = \bar{\mathbf{X}}_\star$, *i.e.*, $\bar{\mathbf{C}}_\star$ is an $r \times k$ matrix with unit-norm columns such that for all $j \in \{1, \dots, k\}$,

$$\bar{\mathbf{X}}_\star^j \top \bar{\mathbf{A}} \bar{\mathbf{X}}_\star^j = \langle \bar{\mathbf{\Lambda}}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_\star^j, \bar{\mathbf{C}}_\star^j \rangle^2. \quad (23)$$

Algorithm 1 iterates over the points ($r \times k$ matrices) \mathbf{C} in $\mathcal{N}_{\epsilon/2}^{\otimes k}(\mathbb{S}_2^{r-1})$, the k th cartesian power of a finite $\epsilon/2$ -net of the r -dimensional l_2 -unit sphere. At each such point \mathbf{C} , it computes a candidate

$$\tilde{\mathbf{X}} = \arg \max_{\mathbf{X} \in \mathcal{X}} \sum_{j=1}^k \langle \mathbf{X}^j, \mathbf{U} \bar{\mathbf{\Lambda}}^{1/2} \mathbf{C}^j \rangle^2$$

via Algorithm 2 (See Lemma 9.1 for the guarantees of Algorithm 2). By construction, the set $\mathcal{N}_{\epsilon/2}^{\otimes k}(\mathbb{S}_2^{r-1})$ contains a \mathbf{C}_\sharp such that

$$\|\mathbf{C}_\sharp - \bar{\mathbf{C}}_\star\|_{\infty, 2} = \max_{j \in \{1, \dots, k\}} \|\mathbf{C}_\sharp^j - \bar{\mathbf{C}}_\star^j\|_2 \leq \epsilon/2. \quad (24)$$

Based on the above, for all $j \in \{1, \dots, k\}$,

$$\begin{aligned}
(\bar{\mathbf{X}}_*^j \bar{\mathbf{A}} \bar{\mathbf{X}}_*^j)^{1/2} &= |\langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, \bar{\mathbf{C}}_*^j \rangle| \\
&= |\langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, \mathbf{C}_\#^j \rangle + \langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, (\bar{\mathbf{C}}_*^j - \mathbf{C}_\#^j) \rangle| \\
&\leq |\langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, \mathbf{C}_\#^j \rangle| + |\langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, (\bar{\mathbf{C}}_*^j - \mathbf{C}_\#^j) \rangle| \\
&\leq |\langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, \mathbf{C}_\#^j \rangle| + \|\bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j\| \cdot \|\bar{\mathbf{C}}_*^j - \mathbf{C}_\#^j\| \\
&\leq |\langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, \mathbf{C}_\#^j \rangle| + (\epsilon/2) \cdot (\bar{\mathbf{X}}_*^j \bar{\mathbf{A}} \bar{\mathbf{X}}_*^j)^{1/2}.
\end{aligned} \tag{25}$$

The first step follows by the definition of $\bar{\mathbf{C}}_*$, the second by the linearity of the inner product, the third by the triangle inequality, the fourth by Cauchy-Schwarz inequality and the last by (24). Rearranging the terms in (25),

$$|\langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, \mathbf{C}_\#^j \rangle| \geq (1 - \frac{\epsilon}{2}) \cdot (\bar{\mathbf{X}}_*^j \bar{\mathbf{A}} \bar{\mathbf{X}}_*^j)^{1/2} \geq 0,$$

and in turn,

$$\langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, \mathbf{C}_\#^j \rangle^2 \geq (1 - \frac{\epsilon}{2})^2 \cdot \bar{\mathbf{X}}_*^j \bar{\mathbf{A}} \bar{\mathbf{X}}_*^j \geq (1 - \epsilon) \cdot \bar{\mathbf{X}}_*^j \bar{\mathbf{A}} \bar{\mathbf{X}}_*^j \tag{26}$$

Summing the terms in (26) over all $j \in \{1, \dots, k\}$,

$$\sum_{j=1}^k \langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_*^j, \mathbf{C}_\#^j \rangle^2 \geq (1 - \epsilon) \cdot \text{Tr}(\bar{\mathbf{X}}_* \bar{\mathbf{A}} \bar{\mathbf{X}}_*). \tag{27}$$

Let $\mathbf{X}_\# \in \mathcal{X}$ be the candidate solution produced by the algorithm at $\mathbf{C}_\#$, *i.e.*,

$$\mathbf{X}_\# \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}} \sum_{j=1}^k \langle \mathbf{x}_j, \bar{\mathbf{U}} \bar{\Lambda}^{1/2} \mathbf{C}_\#^j \rangle^2. \tag{28}$$

Then,

$$\begin{aligned}
\text{Tr}(\mathbf{X}_\# \bar{\mathbf{A}} \mathbf{X}_\#) &\stackrel{(\alpha)}{=} \max_{\mathbf{C}: \mathbf{C}^j \in \mathbb{S}_2^{r-1} \forall j} \sum_{j=1}^k \langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_\#^j, \mathbf{C}^j \rangle^2 \\
&\stackrel{(\beta)}{\geq} \sum_{j=1}^k \langle \bar{\Lambda}^{1/2} \bar{\mathbf{U}}^\top \bar{\mathbf{X}}_\#^j, \mathbf{C}_\#^j \rangle^2 \\
&\stackrel{(\gamma)}{\geq} \sum_{j=1}^k \langle \bar{\mathbf{X}}_*^j, \bar{\mathbf{U}} \bar{\Lambda}^{1/2} \mathbf{C}_\#^j \rangle^2 \\
&\stackrel{(\delta)}{\geq} (1 - \epsilon) \cdot \text{Tr}(\bar{\mathbf{X}}_* \bar{\mathbf{A}} \bar{\mathbf{X}}_*),
\end{aligned} \tag{29}$$

where (α) follows from the observation in (22), (β) from the sub-optimality of $\mathbf{C}_\#$, (γ) by the definition of $\mathbf{X}_\#$ in (28), while (δ) follows from (27). According to (29), at least one of the candidate solutions produced by Algorithm 1, namely $\mathbf{X}_\#$, achieves an objective value within a multiplicative factor $(1 - \epsilon)$ from the optimal, implying the guarantees of the lemma.

Finally, the running time of Algorithm 1 follows immediately from the cost per iteration and the cardinality of the $\epsilon/2$ -net on the unit-sphere. Note that matrix multiplications can exploit the singular value decomposition which is performed once. \square

Theorem 1. For any real $d \times d$ rank- r PSD matrix $\bar{\mathbf{A}}$, desired number of components k , number s of nonzero entries per component, and accuracy parameter $\epsilon \in (0, 1)$, Algorithm 1 outputs $\bar{\mathbf{X}} \in \mathcal{X}_k$ such that

$$\text{Tr}(\bar{\mathbf{X}}^\top \bar{\mathbf{A}} \bar{\mathbf{X}}) \geq (1 - \epsilon) \cdot \text{Tr}(\mathbf{X}_*^\top \bar{\mathbf{A}} \mathbf{X}_*),$$

where $\mathbf{X}_* \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}_k} \text{Tr}(\mathbf{X}^\top \bar{\mathbf{A}} \mathbf{X})$, in time $T_{\text{SVD}}(r) + O\left(\left(\frac{d}{\epsilon}\right)^{r \cdot k} \cdot d \cdot (s \cdot k)^2\right)$. $T_{\text{SVD}}(r)$ is the time required to compute the truncated SVD of $\bar{\mathbf{A}}$.

Proof. Recall that \mathcal{X}_k is the set of $d \times k$ matrices \mathbf{X} whose columns have unit length and pairwise disjoint supports. Algorithm 2, given any $\mathbf{W} \in \mathbb{R}^{d \times k}$, computes $\mathbf{X} \in \mathcal{X}_k$ that optimally solves the constrained maximization in line 5. (See Lemma 9.1 for the guarantee of Algorithm 2). in time $O(d \cdot (s \cdot k)^2)$. The desired result then follows by Lemma 9.2 for the constrained set \mathcal{X}_k . \square

9.3 Guarantees of Algorithm 3 – Proof of Theorem 2

We prove Theorem 2 with the approximation guarantees of Algorithm 3.

Lemma 9.3. For any $d \times d$ PSD matrices \mathbf{A} and $\bar{\mathbf{A}}$, and any set $\mathcal{X} \subseteq \mathbb{R}^{d \times k}$ let

$$\mathbf{X}_* \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}} \text{Tr}(\mathbf{X}^\top \mathbf{A} \mathbf{X}), \quad \text{and} \quad \bar{\mathbf{X}}_* \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}} \text{Tr}(\mathbf{X}^\top \bar{\mathbf{A}} \mathbf{X}).$$

Then, for any $\bar{\mathbf{X}} \in \mathcal{X}$ such that $\text{Tr}(\bar{\mathbf{X}}^\top \bar{\mathbf{A}} \bar{\mathbf{X}}) \geq \gamma \cdot \text{Tr}(\bar{\mathbf{X}}_*^\top \bar{\mathbf{A}} \bar{\mathbf{X}}_*)$ for some $0 < \gamma < 1$,

$$\text{Tr}(\bar{\mathbf{X}}^\top \mathbf{A} \bar{\mathbf{X}}) \geq \gamma \cdot \text{Tr}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*) - 2 \cdot \|\mathbf{A} - \bar{\mathbf{A}}\|_2 \cdot \max_{\mathbf{X} \in \mathcal{X}} \|\mathbf{X}\|_{\text{F}}^2.$$

Proof. By the optimality of $\bar{\mathbf{X}}_*$ for $\bar{\mathbf{A}}$,

$$\text{Tr}(\bar{\mathbf{X}}_*^\top \bar{\mathbf{A}} \bar{\mathbf{X}}_*) \geq \text{Tr}(\mathbf{X}_*^\top \bar{\mathbf{A}} \mathbf{X}_*).$$

In turn, for any $\bar{\mathbf{X}} \in \mathcal{X}$ such that $\text{Tr}(\bar{\mathbf{X}}^\top \bar{\mathbf{A}} \bar{\mathbf{X}}) \geq \gamma \cdot \text{Tr}(\bar{\mathbf{X}}_*^\top \bar{\mathbf{A}} \bar{\mathbf{X}}_*)$ for some $0 < \gamma < 1$,

$$\text{Tr}(\bar{\mathbf{X}}^\top \bar{\mathbf{A}} \bar{\mathbf{X}}) \geq \gamma \cdot \text{Tr}(\mathbf{X}_*^\top \bar{\mathbf{A}} \mathbf{X}_*). \quad (30)$$

Let $\mathbf{E} \triangleq \mathbf{A} - \bar{\mathbf{A}}$. By the linearity of the trace,

$$\begin{aligned} \text{Tr}(\bar{\mathbf{X}}^\top \bar{\mathbf{A}} \bar{\mathbf{X}}) &= \text{Tr}(\bar{\mathbf{X}}^\top \mathbf{A} \bar{\mathbf{X}}) - \text{Tr}(\bar{\mathbf{X}}^\top \mathbf{E} \bar{\mathbf{X}}) \\ &\leq \text{Tr}(\bar{\mathbf{X}}^\top \mathbf{A} \bar{\mathbf{X}}) + |\text{Tr}(\bar{\mathbf{X}}^\top \mathbf{E} \bar{\mathbf{X}})|. \end{aligned} \quad (31)$$

By Lemma 10.10,

$$|\text{Tr}(\bar{\mathbf{X}}^\top \mathbf{E} \bar{\mathbf{X}})| \leq \|\bar{\mathbf{X}}\|_{\text{F}} \cdot \|\bar{\mathbf{X}}\|_{\text{F}} \cdot \|\mathbf{E}\|_2 \leq \|\mathbf{E}\|_2 \cdot \max_{\mathbf{X} \in \mathcal{X}} \|\mathbf{X}\|_{\text{F}}^2 \triangleq R. \quad (32)$$

Continuing from (31),

$$\text{Tr}(\bar{\mathbf{X}}^\top \bar{\mathbf{A}} \bar{\mathbf{X}}) \leq \text{Tr}(\bar{\mathbf{X}}^\top \mathbf{A} \bar{\mathbf{X}}) + R. \quad (33)$$

Similarly,

$$\begin{aligned}
\mathrm{Tr}(\mathbf{X}_*^\top \bar{\mathbf{A}} \mathbf{X}_*) &= \mathrm{Tr}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*) - \mathrm{Tr}(\mathbf{X}_*^\top \mathbf{E} \mathbf{X}_*) \\
&\geq \mathrm{Tr}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*) - |\mathrm{Tr}(\mathbf{X}_*^\top \mathbf{E} \mathbf{X}_*)| \\
&\geq \mathrm{Tr}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*) - R.
\end{aligned} \tag{34}$$

Combining the above, we have

$$\begin{aligned}
\mathrm{Tr}(\bar{\mathbf{X}}^\top \mathbf{A} \bar{\mathbf{X}}) &\geq \mathrm{Tr}(\bar{\mathbf{X}}^\top \bar{\mathbf{A}} \bar{\mathbf{X}}) - R \\
&\geq \gamma \cdot \mathrm{Tr}(\mathbf{X}_*^\top \bar{\mathbf{A}} \mathbf{X}_*) - R \\
&\geq \gamma \cdot (\mathrm{Tr}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*) - R) - R \\
&= \gamma \cdot \mathrm{Tr}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*) - (1 + \gamma) \cdot R \\
&\geq \gamma \cdot \mathrm{Tr}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*) - 2 \cdot R,
\end{aligned}$$

where the first inequality follows from (33) the second from (30), the third from (34), and the last from the fact that $R \geq 0$ and $0 < \gamma \leq 1$. This concludes the proof. \square

Remark 9.2. *If in Lemma 9.3 the PSD matrices \mathbf{A} and $\bar{\mathbf{A}} \in \mathbb{R}^{d \times d}$ are such that $\mathbf{A} - \bar{\mathbf{A}}$ is also PSD, then the following tighter bound holds:*

$$\mathrm{Tr}(\bar{\mathbf{X}}^\top \mathbf{A} \bar{\mathbf{X}}) \geq \gamma \cdot \mathrm{Tr}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*) - \sum_{i=1}^k \lambda_i(\mathbf{A} - \bar{\mathbf{A}}).$$

Proof. This follows from the fact that if $\mathbf{E} \triangleq \mathbf{A} - \bar{\mathbf{A}}$ is PSD, then

$$\mathrm{Tr}(\bar{\mathbf{X}}^\top \mathbf{E} \bar{\mathbf{X}}) = \sum_{j=1}^d \mathbf{x}_j^\top \mathbf{E} \mathbf{x}_j \geq 0,$$

and the bound in (31) can be improved to

$$\mathrm{Tr}(\bar{\mathbf{X}}^\top \bar{\mathbf{A}} \bar{\mathbf{X}}) = \mathrm{Tr}(\bar{\mathbf{X}}^\top \mathbf{A} \bar{\mathbf{X}}) - \mathrm{Tr}(\bar{\mathbf{X}}^\top \mathbf{E} \bar{\mathbf{X}}) \leq \mathrm{Tr}(\bar{\mathbf{X}}^\top \mathbf{A} \bar{\mathbf{X}}).$$

Further, by Lemma 10.11, the bound in (32) can be improved to

$$\mathrm{Tr}(\bar{\mathbf{X}}^\top \mathbf{E} \bar{\mathbf{X}}) \leq \sum_{i=1}^k \lambda_i(\mathbf{E}) \triangleq R.$$

The rest of the proof follows as is. \square

Theorem 2. *For any $n \times d$ input data matrix \mathbf{S} , with corresponding empirical covariance matrix $\mathbf{A} = 1/n \cdot \mathbf{S}^\top \mathbf{S}$, any desired number of components k , and accuracy parameters $\epsilon \in (0, 1)$ and r , Algorithm 3 outputs $\mathbf{X}_{(r)} \in \mathcal{X}_k$ such that*

$$\mathrm{Tr}(\mathbf{X}_{(r)}^\top \mathbf{A} \mathbf{X}_{(r)}) \geq (1 - \epsilon) \cdot \mathrm{Tr}(\mathbf{X}_*^\top \mathbf{A} \mathbf{X}_*) - 2 \cdot k \cdot \|\mathbf{A} - \bar{\mathbf{A}}\|_2,$$

where $\mathbf{X}_* \triangleq \arg \max_{\mathbf{X} \in \mathcal{X}_k} \mathrm{Tr}(\mathbf{X}^\top \mathbf{A} \mathbf{X})$, in time $T_{\text{SKETCH}}(r) + T_{\text{SVD}}(r) + O\left(\left(\frac{4}{\epsilon}\right)^{r \cdot k} \cdot d \cdot (s \cdot k)^2\right)$.

Proof. The theorem follows from Lemma 9.3 and the approximation guarantees of Algorithm 1. \square

9.4 Proof of Theorem 3

First, we restate and prove the following Lemma by [31].

Lemma 9.4. *Let $\mathbf{A} \in \mathbb{R}^{d \times d}$ be an positive semidefinite matrix with entries in $[-1, 1]$, and $\mathbf{V} \in \mathbb{R}^{d \times d}$ matrix such that $\mathbf{A} = \mathbf{V}\mathbf{V}^\top$. Consider a random matrix $\mathbf{R} \in \mathbb{R}^{d \times r}$ with entries drawn according to a Gaussian distribution $N(0, 1/r)$, and define*

$$\bar{\mathbf{A}} = \mathbf{V}\mathbf{R}\mathbf{R}^\top\mathbf{V}^\top.$$

Then, for $r = O(\epsilon^{-2} \log d)$,

$$|[\mathbf{A}]_{i,j} - [\bar{\mathbf{A}}]_{i,j}| \leq \epsilon$$

for all i, j with probability at least $1 - 1/d$.

Proof. The proof relies on the Johnson-Lindenstrauss (JL) Lemma [38], according to which for any two unit norm vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ and \mathbf{R} generated as described

$$\Pr\{|\mathbf{x}^\top \mathbf{R}\mathbf{R}^\top \mathbf{y} - \mathbf{x}^\top \mathbf{y}| \geq \epsilon\} \leq 2 \cdot e^{-(\epsilon^2 - \epsilon^3) \cdot r/4}.$$

Observe that each element of \mathbf{A} is in $[-1, 1]$, hence can be rewritten as an inner product of two unit-norm vectors:

$$[\mathbf{A}]_{i,j} = \mathbf{V}_{:,i}^\top \mathbf{V}_{:,j}.$$

Setting $r = O(\epsilon^{-2} \log d)$ and using the JL lemma and a union bound over all $O(d^2)$ vector pairs $\mathbf{V}_{:,i}, \mathbf{V}_{:,j}$ we obtain the desired result. \square

Next, we provide the proof of Theorem 3 for the simple case of $k = 1$; the proof easily generalizes to the multi-component case $k > 1$. According to Lemma 9.4, choosing $d = O((\delta/6)^{-2} \log n) = O(\delta^{-2} \log n)$ suffices for all entries of $\bar{\mathbf{A}}$ constructed as described in the lemma to satisfy

$$|[\mathbf{A}]_{i,j} - [\bar{\mathbf{A}}]_{i,j}| \leq \frac{\delta}{6}$$

with probability at least $1 - 1/d$. In turn, for any s -sparse, unit-norm \mathbf{x} ,

$$\begin{aligned} |\mathbf{x}^\top \mathbf{A}\mathbf{x} - \mathbf{x}^\top \bar{\mathbf{A}}\mathbf{x}| &= \left| \sum_{i,j} x_i x_j ([\mathbf{A}]_{ij} - [\bar{\mathbf{A}}]_{ij}) \right| \leq \frac{\delta}{6} \cdot \left| \sum_{i=1}^n |x_i| \sum_{j=1}^n |x_j| \right| \\ &\leq \frac{\delta}{6} \cdot \|\mathbf{x}\|_1^2 \leq \frac{\delta}{6} \cdot (\sqrt{s} \cdot \|\mathbf{x}\|_2)^2 = \frac{\delta}{6} \cdot s, \end{aligned} \quad (35)$$

where the second inequality follows from the fact that \mathbf{x} is s -sparse and unit norm.

We run Algorithm 1 (for $k = 1$) with input argument the rank- r matrix $\bar{\mathbf{A}}$, desired sparsity s and accuracy parameter $\epsilon = \delta/6$. Algorithm 1 outputs a s -sparse unit-norm vector $\hat{\mathbf{x}}$ which according to Theorem 1 satisfies

$$(1 - \delta/6) \cdot \mathbf{x}_d^\top \bar{\mathbf{A}}\mathbf{x}_d \leq \hat{\mathbf{x}}^\top \bar{\mathbf{A}}\hat{\mathbf{x}} \leq \mathbf{x}_d^\top \bar{\mathbf{A}}\mathbf{x}_d, \quad (36)$$

where \mathbf{x}_d is the true s -sparse principal component of $\bar{\mathbf{A}}$. This, in turn, implies that $\hat{\mathbf{x}}$ satisfies

$$\left| \hat{\mathbf{x}}^\top \bar{\mathbf{A}}\hat{\mathbf{x}} - \mathbf{x}_d^\top \bar{\mathbf{A}}\mathbf{x}_d \right| \leq \frac{\delta}{6} \cdot \mathbf{x}_d^\top \bar{\mathbf{A}}\mathbf{x}_d \leq \frac{\delta}{6} \left(1 + \frac{\delta}{6} \right) s \leq \frac{\delta}{3} \cdot s, \quad (37)$$

where the second inequality follows from the fact that the entries of $\bar{\mathbf{A}}$ lie in $[-1 - \frac{\delta}{6}, 1 + \frac{\delta}{6}]$ and $\hat{\mathbf{x}}$ is s -sparse and unit-norm.

In the following, we bound the difference of the performance of $\hat{\mathbf{x}}$ on the original matrix \mathbf{A} from the optimal value. Let \mathbf{x}_* denote the s -sparse principal component of \mathbf{A} and define

$$\text{OPT} \triangleq \mathbf{x}_*^T \mathbf{A} \mathbf{x}_*.$$

Then,

$$\begin{aligned} |\text{OPT} - \hat{\mathbf{x}}^T \mathbf{A} \hat{\mathbf{x}}| &= |\mathbf{x}_*^T \mathbf{A} \mathbf{x}_* - \hat{\mathbf{x}}^T \mathbf{A} \hat{\mathbf{x}}| \\ &= |\mathbf{x}_*^T \mathbf{A} \mathbf{x}_* - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d + \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \hat{\mathbf{x}}^T \mathbf{A} \hat{\mathbf{x}}| \\ &\leq \underbrace{|\mathbf{x}_*^T \mathbf{A} \mathbf{x}_* - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d|}_A + \underbrace{|\mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \hat{\mathbf{x}}^T \mathbf{A} \hat{\mathbf{x}}|}_B. \end{aligned} \quad (38)$$

Utilizing (35) and the triangle inequality, one can verify that

$$\begin{aligned} A &= |\mathbf{x}_*^T \mathbf{A} \mathbf{x}_* - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d + \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d| \\ &\leq |\mathbf{x}_*^T \mathbf{A} \mathbf{x}_* - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d| + |\mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d| \\ &\leq \underbrace{|\mathbf{x}_*^T \mathbf{A} \mathbf{x}_* - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d|}_{\geq 0} + \frac{\delta}{6} \cdot s \\ &\leq \mathbf{x}_*^T \mathbf{A} \mathbf{x}_* - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d + \frac{\delta}{6} \cdot s + \underbrace{|\mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \mathbf{x}_*^T \bar{\mathbf{A}} \mathbf{x}_*|}_{\geq 0} \\ &\leq \mathbf{x}_*^T \mathbf{A} \mathbf{x}_* - \mathbf{x}_*^T \bar{\mathbf{A}} \mathbf{x}_* + \frac{\delta}{6} \cdot s + \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d \\ &\leq |\mathbf{x}_*^T \mathbf{A} \mathbf{x}_* - \mathbf{x}_*^T \bar{\mathbf{A}} \mathbf{x}_*| + \frac{\delta}{6} \cdot s + |\mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d| \\ &\leq \frac{\delta}{2} \cdot s. \end{aligned} \quad (39)$$

Similarly,

$$\begin{aligned} B &= |\mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \hat{\mathbf{x}}^T \bar{\mathbf{A}} \hat{\mathbf{x}} + \hat{\mathbf{x}}^T \bar{\mathbf{A}} \hat{\mathbf{x}} - \hat{\mathbf{x}}^T \mathbf{A} \hat{\mathbf{x}}| \\ &= |\mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \hat{\mathbf{x}}^T \bar{\mathbf{A}} \hat{\mathbf{x}}| + |\hat{\mathbf{x}}^T \bar{\mathbf{A}} \hat{\mathbf{x}} - \hat{\mathbf{x}}^T \mathbf{A} \hat{\mathbf{x}}| \\ &\leq |\mathbf{x}_d^T \bar{\mathbf{A}} \mathbf{x}_d - \hat{\mathbf{x}}^T \bar{\mathbf{A}} \hat{\mathbf{x}}| + \frac{\delta}{6} \cdot s \\ &\stackrel{(\alpha)}{\leq} \frac{2\delta}{6} \cdot s + \frac{\delta}{6} \cdot s \\ &\leq \frac{\delta}{2} \cdot s. \end{aligned} \quad (40)$$

where (α) follows from (37). Continuing from (38), combining (39) and (40) we obtain

$$|\text{OPT} - \hat{\mathbf{x}}^T \mathbf{A} \hat{\mathbf{x}}| \leq \delta \cdot s,$$

which is the desired result. ■

10 Auxiliary Technical Lemmata

Lemma 10.5. For any real $d \times n$ matrix \mathbf{M} , and any $r, k \leq \min\{d, n\}$,

$$\sum_{i=r+1}^{r+k} \sigma_i(\mathbf{M}) \leq \frac{k}{\sqrt{r+k}} \cdot \|\mathbf{M}\|_{\mathbb{F}},$$

where $\sigma_i(\mathbf{M})$ is the i th largest singular value of \mathbf{M} .

Proof. By the Cauchy-Schwartz inequality,

$$\sum_{i=r+1}^{r+k} \sigma_i(\mathbf{M}) = \sum_{i=r+1}^{r+k} |\sigma_i(\mathbf{M})| \leq \left(\sum_{i=r+1}^{r+k} \sigma_i^2(\mathbf{M}) \right)^{1/2} \cdot \|\mathbf{1}_k\|_2 = \sqrt{k} \cdot \left(\sum_{i=r+1}^{r+k} \sigma_i^2(\mathbf{M}) \right)^{1/2}.$$

Note that $\sigma_{r+1}(\mathbf{M}), \dots, \sigma_{r+k}(\mathbf{M})$ are the k smallest among the $r+k$ largest singular values. Hence,

$$\sum_{i=r+1}^{r+k} \sigma_i^2(\mathbf{M}) \leq \frac{k}{r+k} \sum_{i=1}^{r+k} \sigma_i^2(\mathbf{M}) \leq \frac{k}{r+k} \sum_{i=1}^{\min\{d,n\}} \sigma_i^2(\mathbf{M}) = \frac{k}{r+k} \|\mathbf{M}\|_{\mathbb{F}}^2.$$

Combining the two inequalities, the desired result follows. \square

Corollary 1. For any real $d \times n$ matrix \mathbf{M} and $k \leq \min\{d, n\}$, $\sigma_k(\mathbf{M}) \leq k^{-1/2} \cdot \|\mathbf{M}\|_{\mathbb{F}}$.

Proof. It follows immediately from Lemma 10.5. \square

Lemma 10.6. Let a_1, \dots, a_n and b_1, \dots, b_n be $2n$ real numbers and let p and q be two numbers such that $1/p + 1/q = 1$ and $p > 1$. We have

$$\left| \sum_{i=1}^n a_i b_i \right| \leq \left(\sum_{i=1}^n |a_i|^p \right)^{1/p} \cdot \left(\sum_{i=1}^n |b_i|^q \right)^{1/q}.$$

Lemma 10.7. For any two real matrices \mathbf{A} and \mathbf{B} of appropriate dimensions,

$$\|\mathbf{AB}\|_{\mathbb{F}} \leq \min\{\|\mathbf{A}\|_2 \|\mathbf{B}\|_{\mathbb{F}}, \|\mathbf{A}\|_{\mathbb{F}} \|\mathbf{B}\|_2\}.$$

Proof. Let \mathbf{b}_i denote the i th column of \mathbf{B} . Then,

$$\|\mathbf{AB}\|_{\mathbb{F}}^2 = \sum_i \|\mathbf{A}\mathbf{b}_i\|_2^2 \leq \sum_i \|\mathbf{A}\|_2^2 \|\mathbf{b}_i\|_2^2 = \|\mathbf{A}\|_2^2 \sum_i \|\mathbf{b}_i\|_2^2 = \|\mathbf{A}\|_2^2 \|\mathbf{B}\|_{\mathbb{F}}^2.$$

Similarly, using the previous inequality,

$$\|\mathbf{AB}\|_{\mathbb{F}}^2 = \|\mathbf{B}^{\top} \mathbf{A}^{\top}\|_{\mathbb{F}}^2 \leq \|\mathbf{B}^{\top}\|_2^2 \|\mathbf{A}^{\top}\|_{\mathbb{F}}^2 = \|\mathbf{B}\|_2^2 \|\mathbf{A}\|_{\mathbb{F}}^2.$$

Combining the two upper bounds, the desired result follows. \square

Lemma 10.8. For any $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n \times k}$,

$$|\langle \mathbf{A}, \mathbf{B} \rangle| \triangleq |\text{Tr}(\mathbf{A}^{\top} \mathbf{B})| \leq \|\mathbf{A}\|_{\mathbb{F}} \|\mathbf{B}\|_{\mathbb{F}}.$$

Proof. The inequality follows from Lemma 10.6 for $p = q = 2$, treating \mathbf{A} and \mathbf{B} as vectors. \square

Lemma 10.9. For any real $m \times n$ matrix \mathbf{A} , and any $k \leq \min\{m, n\}$,

$$\max_{\substack{\mathbf{Y} \in \mathbb{R}^{n \times k} \\ \mathbf{Y}^\top \mathbf{Y} = \mathbf{I}_k}} \|\mathbf{A}\mathbf{Y}\|_{\text{F}} = \left(\sum_{i=1}^k \sigma_i^2(\mathbf{A}) \right)^{1/2}.$$

The maximum is attained by \mathbf{Y} coinciding with the k leading right singular vectors of \mathbf{A} .

Proof. Let $\mathbf{U}\Sigma\mathbf{V}^\top$ be the singular value decomposition of \mathbf{A} ; \mathbf{U} and \mathbf{V} are $m \times m$ and $n \times n$ unitary matrices respectively, while Σ is a diagonal matrix with $\Sigma_{jj} = \sigma_j$, the j th largest singular value of \mathbf{A} , $j = 1, \dots, d$, where $d \triangleq \min\{m, n\}$. Due to the invariance of the Frobenius norm under unitary multiplication,

$$\|\mathbf{A}\mathbf{Y}\|_{\text{F}}^2 = \|\mathbf{U}\Sigma\mathbf{V}^\top \mathbf{Y}\|_{\text{F}}^2 = \|\Sigma\mathbf{V}^\top \mathbf{Y}\|_{\text{F}}^2. \quad (41)$$

Continuing from (41),

$$\|\Sigma\mathbf{V}^\top \mathbf{Y}\|_{\text{F}}^2 = \text{Tr}\left(\mathbf{Y}^\top \mathbf{V}\Sigma^2 \mathbf{V}^\top \mathbf{Y}\right) = \sum_{i=1}^k \mathbf{y}_i^\top \left(\sum_{j=1}^d \sigma_j^2 \cdot \mathbf{v}_j \mathbf{v}_j^\top \right) \mathbf{y}_i = \sum_{j=1}^d \sigma_j^2 \cdot \sum_{i=1}^k \left(\mathbf{v}_j^\top \mathbf{y}_i \right)^2.$$

Let $z_j \triangleq \sum_{i=1}^k \left(\mathbf{v}_j^\top \mathbf{y}_i \right)^2$, $j = 1, \dots, d$. Note that each individual z_j satisfies

$$0 \leq z_j \triangleq \sum_{i=1}^k \left(\mathbf{v}_j^\top \mathbf{y}_i \right)^2 \leq \|\mathbf{v}_j\|^2 = 1,$$

where the last inequality follows from the fact that the columns of \mathbf{Y} are orthonormal. Further,

$$\sum_{j=1}^d z_j = \sum_{j=1}^d \sum_{i=1}^k \left(\mathbf{v}_j^\top \mathbf{y}_i \right)^2 = \sum_{i=1}^k \sum_{j=1}^d \left(\mathbf{v}_j^\top \mathbf{y}_i \right)^2 = \sum_{i=1}^k \|\mathbf{y}_i\|^2 = k.$$

Combining the above, we conclude that

$$\|\mathbf{A}\mathbf{Y}\|_{\text{F}}^2 = \sum_{j=1}^d \sigma_j^2 \cdot z_j \leq \sigma_1^2 + \dots + \sigma_k^2. \quad (42)$$

Finally, it is straightforward to verify that if $\mathbf{y}_i = \mathbf{v}_i$, $i = 1, \dots, k$, then (42) holds with equality. \square

Lemma 10.10. For any real $d \times n$ matrix \mathbf{A} , and pair of $d \times k$ matrix \mathbf{X} and $n \times k$ matrix \mathbf{Y} such that $\mathbf{X}^\top \mathbf{X} = \mathbf{I}_k$ and $\mathbf{Y}^\top \mathbf{Y} = \mathbf{I}_k$ with $k \leq \min\{d, n\}$, the following holds:

$$|\text{Tr}(\mathbf{X}^\top \mathbf{A}\mathbf{Y})| \leq \sqrt{k} \cdot \left(\sum_{i=1}^k \sigma_i^2(\mathbf{A}) \right)^{1/2}.$$

Proof. By Lemma 10.8,

$$|\langle \mathbf{X}, \mathbf{A}\mathbf{Y} \rangle| = |\text{Tr}(\mathbf{X}^\top \mathbf{A}\mathbf{Y})| \leq \|\mathbf{X}\|_{\text{F}} \cdot \|\mathbf{A}\mathbf{Y}\|_{\text{F}} = \sqrt{k} \cdot \|\mathbf{A}\mathbf{Y}\|_{\text{F}}$$

where the last inequality follows from the fact that $\|\mathbf{X}\|_{\text{F}}^2 = \text{Tr}(\mathbf{X}^\top \mathbf{X}) = \text{Tr}(\mathbf{I}_k) = k$. Combining with a bound on $\|\mathbf{A}\mathbf{Y}\|_{\text{F}}$ as in Lemma 10.9, completes the proof. \square

Lemma 10.11. For any real $d \times d$ PSD matrix \mathbf{A} , and $k \times d$ matrix \mathbf{X} with $k \leq d$ orthonormal columns,

$$\text{Tr}(\mathbf{X}^\top \mathbf{A} \mathbf{X}) \leq \sum_{i=1}^k \lambda_i(\mathbf{A})$$

where $\lambda_i(\mathbf{A})$ is the i th largest eigenvalue of \mathbf{A} . Equality is achieved for \mathbf{X} coinciding with the k leading eigenvectors of \mathbf{A} .

Proof. Let $\mathbf{A} = \mathbf{V}\mathbf{V}^\top$ be a factorization of the PSD matrix \mathbf{A} . Then, $\text{Tr}(\mathbf{X}^\top \mathbf{A} \mathbf{X}) = \text{Tr}(\mathbf{X}^\top \mathbf{V}\mathbf{V}^\top \mathbf{X}) = \|\mathbf{V}^\top \mathbf{X}\|_{\text{F}}^2$. The desired result follows by Lemma 10.9 and the fact that $\lambda_i(\mathbf{A}) = \sigma_i^2(\mathbf{V})$, $i = 1, \dots, d$. \square

11 Additional Experimental Results

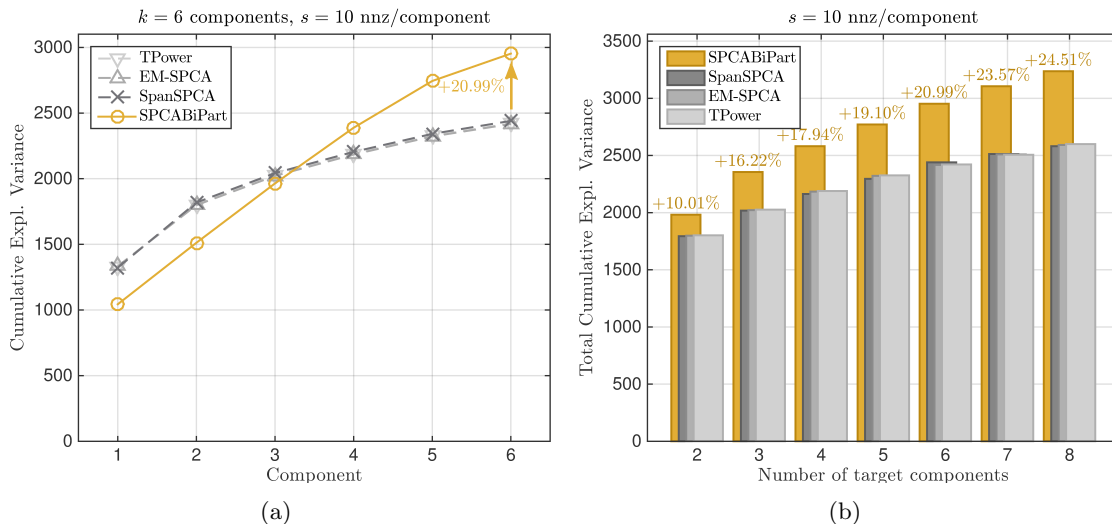


Figure 3: Cumulative variance captured by k s -spars components computed on the word-by-word matrix – BAGOFWORDS:NIPS dataset [37]. Sparsity is arbitrarily set to $s = 10$ nonzero entries per component. Fig. 3(a) depicts the cum. variance captured by $k = 6$ components. Deflation leads to a greedy formation of components; first components capture high variance, but subsequent ones contribute less. On the contrary, our algorithm jointly optimizes the k components and achieves higher total cum. variance. Fig. 3(b) depicts the total cum. variance achieved for various values of k . Our algorithm operates on a rank-4 approximation of the input.

	Topic 1	Topic 2	Topic 3	Topic 4	Topic 5	Topic 6	Topic 7	Topic 8
TPOWER	1: network	algorithm	neuron	parameter	object	classifier	word	noise
	2: model	data	cell	point	image	net	speech	control
	3: learning	system	pattern	distribution	recognition	classification	level	dynamic
	4: input	error	layer	hidden	images	class	context	step
	5: function	weight	information	space	task	test	hmm	term
	6: neural	problem	signal	gaussian	features	order	character	optimal
	7: unit	result	visual	linear	feature	examples	processing	component
	8: set	number	field	probability	representation	rate	non	equation
	9: training	method	synaptic	mean	performance	values	approach	single
	10: output	vector	firing	case	view	experiment	trained	analysis
SPANSPCA	11: network	algorithm	neuron	parameter	recognition	control	classifier	noise
	12: model	data	cell	distribution	object	action	classification	order
	13: input	weight	pattern	point	image	dynamic	class	term
	14: learning	error	layer	linear	word	step	net	component
	15: neural	problem	signal	probability	performance	optimal	test	rate
	16: function	output	information	space	task	policy	speech	equation
	17: unit	result	visual	gaussian	features	states	examples	single
	18: set	number	synaptic	hidden	representation	reinforcement	approach	analysis
	19: system	method	field	case	feature	values	experiment	large
	20: training	vector	response	mean	images	controller	trained	form
SPCABIPART	21: data	function	neuron	unit	learning	network	model	training
	22: distribution	algorithm	cell	weight	space	input	parameter	hidden
	23: gaussian	set	visual	layer	action	neural	information	performance
	24: probability	error	direction	net	order	system	control	recognition
	25: component	problem	firing	task	step	output	dynamic	classifier
	26: approach	result	synaptic	connection	linear	pattern	mean	test
	27: analysis	number	response	activation	case	signal	noise	word
	28: mixture	method	spike	architecture	values	processing	field	speech
	29: likelihood	vector	activity	generalization	term	image	local	classification
	30: experiment	point	motion	threshold	optimal	object	equation	trained

	Total Cum. Variance
TPOWER	$2.5999 \cdot 10^3$
SPANSPCA	$2.5981 \cdot 10^3$
SPCABIPART	$3.2090 \cdot 10^3$

Table 4: BAGOFWORDS:NIPS dataset [37]. We run various SPCA algorithms for $k = 8$ components (topics) and $s = 10$ nonzero entries per component. The table lists the words selected by each component (words corresponding to higher magnitude entries appear higher in the topic). Our algorithm was configured to use a rank-4 approximation of the input data.

	Topic 1	Topic 2	Topic 3	Topic 4	Topic 5	Topic 6	Topic 7	Topic 8
TPOWER	1: percent	zzz_bush	team	school	women	zzz_enron	drug	palestinian
	2: company	zzz_al_gore	game	student	show	firm	patient	zzz_israel
	3: million	president	season	program	book	zzz_arthur_andersen	doctor	zzz_israeli
	4: companies	official	player	high	com	deal	system	zzz_yasser_arafat
	5: market	zzz_george_bush	play	children	look	lay	problem	attack
	6: stock	campaign	games	right	american	financial	law	leader
	7: business	government	point	group	need	energy	care	peace
	8: money	plan	run	home	part	executives	cost	israelis
	9: billion	administration	coach	public	family	accounting	help	israeli
	10: fund	zzz_white_house	win	teacher	found	partnership	health	zzz_west_bank
SPANSPCA	11: percent	team	zzz_bush	palestinian	school	cup	show	won
	12: company	game	zzz_al_gore	attack	student	minutes	com	night
	13: million	season	president	zzz_united_states	children	add	part	left
	14: companies	player	zzz_george_bush	zzz_u_s	program	tablespoon	look	big
	15: market	play	campaign	military	home	teaspoon	need	put
	16: stock	games	official	leader	family	oil	book	win
	17: business	point	government	zzz_israel	women	pepper	called	hit
	18: money	run	political	zzz_american	public	water	hour	job
	19: billion	right	election	war	high	large	american	ago
	20: plan	coach	group	country	law	sugar	help	zzz_new_york
SPCABIPART	21: percent	zzz_united_states	zzz_bush	company	team	cup	school	zzz_al_gore
	22: million	zzz_u_s	official	companies	game	minutes	student	zzz_george_bush
	23: money	zzz_american	government	market	season	add	children	campaign
	24: high	attack	president	stock	player	tablespoon	women	election
	25: program	military	group	business	play	oil	show	plan
	26: number	palestinian	leader	billion	point	teaspoon	book	tax
	27: need	war	country	analyst	run	water	family	public
	28: part	administration	political	firm	right	pepper	look	zzz_washington
	29: problem	zzz_white_house	american	sales	home	large	hour	member
	30: com	games	law	cost	won	food	small	nation

Total Cum. Variance	
TPOWER	45.4014
SPANSPCA	46.0075
SPCABIPART	47.7212

Table 5: BAGOFWORDS:NYTIMES dataset [37]. We run various SPCA algorithms for $k = 8$ components (topics) and $s = 10$ nonzero entries per component. The table lists the words selected by each component (words corresponding to higher magnitude entries appear higher in the topic). Our algorithm was configured to use a rank-4 approximation of the input data.

	Topic 1	Topic 2	Topic 3	Topic 4	Topic 5	Topic 6	Topic 7	Topic 8
TPOWER	1: percent	zzz_bush	team	school	com	zzz_enron	law	palestinian
	2: company	zzz_al_gore	game	student	women	firm	drug	zzz_israel
	3: million	zzz_george_bush	season	program	book	deal	court	zzz_israeli
	4: companies	campaign	player	children	web	financial	case	zzz_yasser_arafat
	5: market	right	play	show	american	zzz_arthur_andersen	federal	peace
	6: stock	group	games	public	information	chief	patient	israelis
	7: money	political	point	need	look	executive	system	israeli
	8: business	zzz_united_states	run	part	site	analyst	decision	military
	9: government	zzz_us	coach	family	zzz_new_york	executives	bill	zzz_palestinian
	10: official	administration	home	help	question	lay	member	zzz_west_bank
	11: billion	leader	win	job	number	investor	lawyer	war
	12: president	attack	won	teacher	called	energy	doctor	security
	13: plan	zzz_white_house	night	country	find	investment	cost	violence
	14: high	tax	left	problem	found	employees	care	killed
	15: fund	zzz_washington	guy	parent	ago	accounting	health	talk
SPANSPCA	16: percent	team	official	zzz_al_gore	cup	show	public	night
	17: company	game	zzz_bush	zzz_george_bush	minutes	com	member	big
	18: million	season	zzz_united_states	campaign	add	part	system	set
	19: companies	player	attack	election	tablespoon	look	case	film
	20: market	play	zzz_us	political	teaspoon	need	number	find
	21: stock	games	palestinian	vote	oil	book	question	room
	22: business	point	military	republican	pepper	women	job	place
	23: money	run	leader	voter	water	family	told	friend
	24: billion	right	zzz_american	democratic	large	called	put	took
	25: plan	win	war	school	sugar	children	zzz_washington	start
	26: government	coach	zzz_israel	presidential	servng	help	found	car
	27: president	home	country	zzz_white_house	butter	ago	information	feel
	28: high	won	administration	law	chopped	zzz_new_york	federal	half
	29: cost	left	terrorist	zzz_republican	hour	program	student	guy
	30: group	hit	american	tax	pan	problem	court	early
SPCABIPART	31: company	show	cup	team	percent	zzz_al_gore	official	school
	32: companies	home	minutes	game	million	zzz_george_bush	zzz_bush	student
	33: stock	run	add	season	money	campaign	government	children
	34: market	com	tablespoon	player	plan	right	president	women
	35: billion	high	oil	play	business	election	zzz_united_states	book
	36: zzz_enron	need	teaspoon	games	tax	political	zzz_us	family
	37: firm	look	pepper	coach	cost	point	group	called
	38: analyst	part	water	guy	cut	leader	attack	hour
	39: industry	night	large	yard	job	zzz_washington	zzz_american	friend
	40: fund	zzz_new_york	sugar	hit	pay	administration	country	found
	41: investor	help	servng	played	deal	question	military	find
	42: sales	left	butter	playing	quarter	member	american	set
	43: customer	put	chopped	ball	chief	won	war	room
	44: investment	ago	fat	fan	executive	win	law	film
	45: economy	big	food	shot	financial	told	public	small

Total Cum. Variance	
TPOWER	48.140645
SPANSPCA	48.767864
SPCABIPART	51.873063

Table 6: BAGOFWORDS:NYTIMES dataset [37]. We run various SPCA algorithms for $k = 8$ components (topics) and cardinality $s = 15$ per component. The table lists the words corresponding to each component (words corresponding to higher magnitude entries appear higher in the topic). Our algorithm was configured to use a rank-4 approximation of the input data.

	Topic 1	Topic 2	Topic 3	Topic 4	Topic 5	Topic 6	Topic 7	Topic 8
TPOWER	1: percent	zzz_bush	team	school	com	zzz_enron	drug	palestinian
	2: company	zzz_al_gore	game	student	women	court	patient	zzz_israel
	3: million	zzz_george_bush	season	program	book	case	doctor	zzz_israeli
	4: companies	campaign	player	children	web	firm	cell	zzz_yasser_arafat
	5: market	zzz_united_states	play	show	site	federal	care	peace
	6: stock	zzz_u_s	games	public	information	lawyer	disease	israelis
	7: government	political	point	part	zzz_new_york	deal	health	israeli
	8: official	attack	run	family	www	decision	medical	zzz_palestinian
	9: money	zzz_american	home	system	hour	chief	test	zzz_west_bank
	10: business	american	coach	help	find	power	hospital	security
	11: president	administration	win	problem	mail	industry	research	violence
	12: billion	leader	won	law	found	executive	cancer	killed
	13: plan	country	left	job	put	according	treatment	talk
	14: group	election	night	called	set	financial	study	meeting
	15: high	zzz_washington	hit	look	room	office	death	soldier
	16: right	military	guy	member	big	analyst	human	minister
	17: fund	zzz_white_house	yard	question	told	executives	heart	zzz_sharon
	18: need	war	played	ago	friend	zzz_arthur_andersen	blood	fire
	19: cost	tax	start	teacher	director	employees	trial	zzz_ariel_sharon
	20: number	nation	playing	parent	place	investor	benefit	zzz_arab
SPANSPCA	21: percent	team	zzz_al_gore	attack	school	cup	com	drug
	22: company	game	zzz_bush	zzz_united_states	student	minutes	web	patient
	23: million	season	zzz_george_bush	zzz_u_s	children	add	site	cell
	24: companies	player	campaign	palestinian	program	tablespoon	information	doctor
	25: market	play	election	military	family	oil	computer	disease
	26: stock	games	political	zzz_american	women	teaspoon	find	care
	27: business	point	tax	zzz_israel	show	pepper	big	health
	28: money	run	republican	war	help	water	zzz_new_york	test
	29: billion	win	zzz_white_house	country	told	large	www	research
	30: government	home	vote	terrorist	parent	sugar	mail	human
	31: president	won	law	american	problem	servng	set	medical
	32: plan	coach	administration	zzz_taliban	book	butter	put	study
	33: high	left	democratic	zzz_afghanistan	job	chopped	director	death
	34: group	night	voter	security	found	hour	industry	cancer
	35: official	hit	leader	zzz_israeli	friend	pan	room	hospital
	36: need	guy	public	nation	ago	fat	small	treatment
	37: right	yard	zzz_republican	member	question	bowl	car	scientist
	38: part	played	presidential	support	teacher	gram	zzz_internet	according
	39: cost	look	federal	called	case	food	place	blood
	40: system	start	zzz_washington	forces	number	medium	film	heart
SPCABIPART	41: palestinian	percent	zzz_al_gore	cup	school	team	company	official
	42: zzz_israel	million	zzz_bush	minutes	right	game	market	government
	43: zzz_israeli	money	zzz_george_bush	add	group	season	companies	president
	44: zzz_yasser_arafat	billion	campaign	tablespoon	show	player	stock	zzz_united_states
	45: peace	business	election	oil	home	play	zzz_enron	zzz_u_s
	46: war	fund	political	teaspoon	high	games	analyst	attack
	47: terrorist	tax	zzz_white_house	pepper	program	point	firm	zzz_american
	48: zzz_taliban	cost	administration	water	need	run	industry	country
	49: zzz_afghanistan	cut	republican	hour	part	coach	investor	law
	50: forces	job	leader	large	com	win	sales	plan
	51: bin	pay	vote	sugar	american	won	customer	public
	52: troop	economy	democratic	serving	look	left	price	zzz_washington
	53: laden	deal	presidential	butter	help	night	investment	member
	54: student	big	zzz_clinton	chopped	problem	hit	quarter	system
	55: zzz_pakistan	chief	support	pan	called	guy	executives	nation
	56: product	executive	zzz_congress	fat	zzz_new_york	yard	consumer	case
	57: zzz_internet	financial	military	bowl	number	played	technology	federal
	58: profit	start	policy	gram	question	ball	share	information
	59: earning	record	court	food	ago	playing	prices	power
	60: shares	manager	security	league	told	lead	growth	effort

Total Cum. Variance	
TPOWER	50.7686
SPANSPCA	52.8117
SPCABIPART	54.8906

Table 7: BAGOFWORDS:NYTIMES dataset [37]. We run various SPCA algorithms for $k = 8$ components (topics) and cardinality $s = 20$ per component. The table lists the words corresponding to each component (words corresponding to higher magnitude entries appear higher in the topic). Our algorithm was configured to use a rank-4 approximation of the input data.

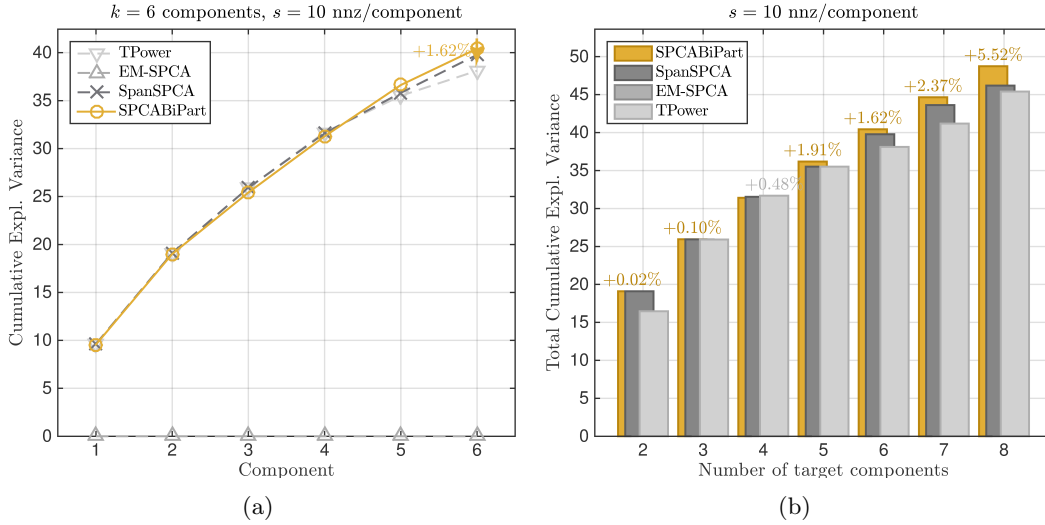


Figure 4: Cumulative variance captured by k s -sparse ($s = 10$) extracted components on the word-by-word matrix – BAGOFWORDS:NYTIMES dataset [37]. Fig. 4(a) depicts the cum. variance captured by $k = 6$ components. Deflation leads to a greedy formation of components; first components capture high variance, but subsequent ones contribute less. On the contrary, our algorithm jointly optimizes the k components and achieves higher total cum. variance. Fig. 4(b) depicts the total cum. variance achieved for various values of k . Sparsity is arbitrarily set to $s = 10$ nonzero entries per component. Our algorithm operates on a rank-4 approximation.

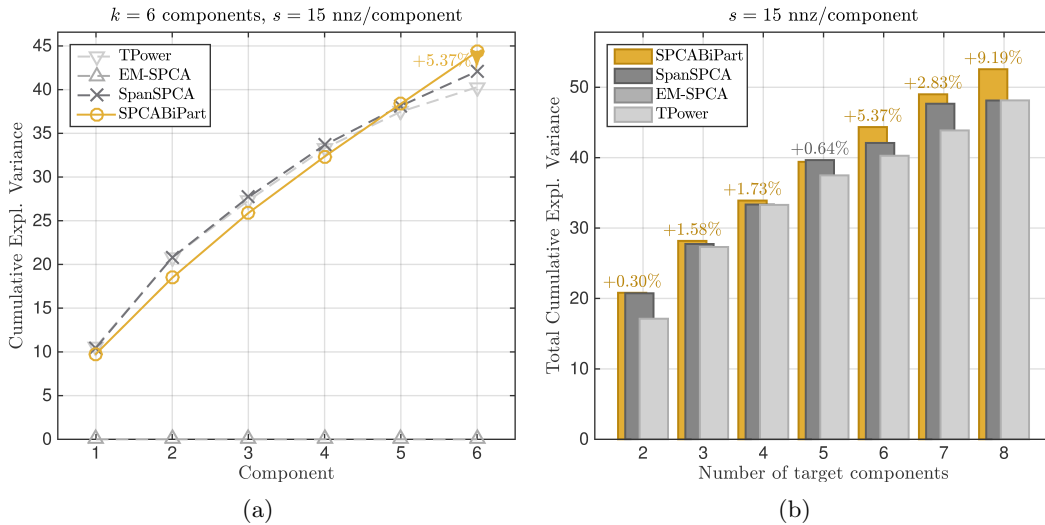


Figure 5: Same as Fig. 4, but for sparsity $s = 15$.

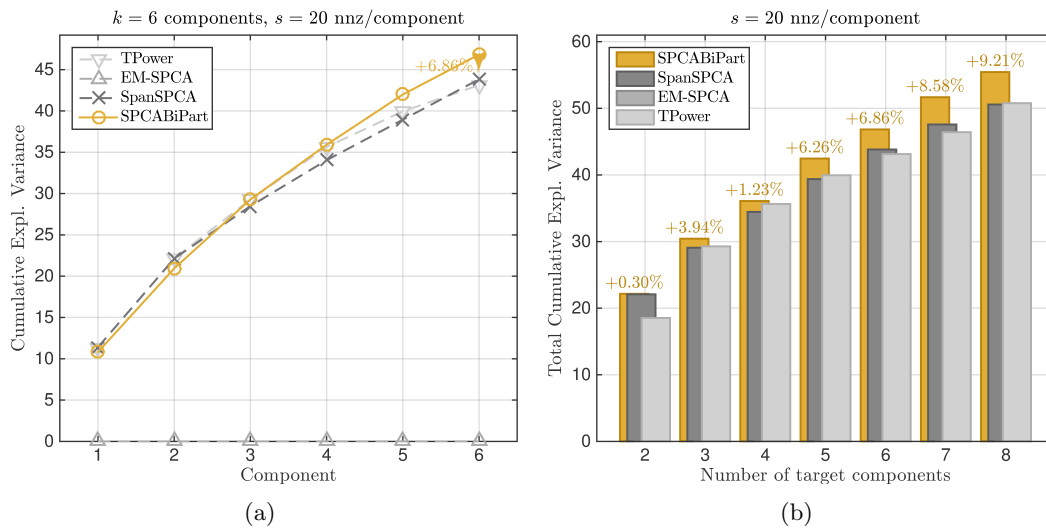


Figure 6: Same as Fig. 4, but for sparsity $s = 20$.