Optimal Sparse Linear Auto-Encoders and Sparse PCA

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Abstract

Principal components analysis (PCA) is the optimal linear auto-encoder of data, and it is often used to construct features. Enforcing sparsity on the principal components can promote better generalization, while improving the interpretability of the features. We study the problem of constructing optimal sparse linear auto-encoders. Two natural questions in such a setting are:

(i) Given a level of sparsity, what is the best approximation to PCA that can be achieved?

(ii) Are there low-order polynomial-time algorithms which can asymptotically achieve this optimal trade-off between the sparsity and the approximation quality?

In this work, we answer both questions by giving efficient low-order polynomial-time algorithms for constructing asymptotically optimal linear auto-encoders (in particular, sparse features with near-PCA reconstruction error) and demonstrate the performance of our algorithms on real data.

1 Introduction

An auto-encoder transforms (encodes) the data into a low dimensional space (the feature space) and then lifts (decodes) it back to the original space. The auto-encoder reconstructs the data through a bottleneck, and if the reconstruction is close to the original data, then the encoder was able to preserve most of the information using just a small number of features. Auto-encoders are important in machine learning because they perform information preserving dimension reduction. The decoder only plays a minor role in verifying that the encoder didn’t lose much information. It is the encoder that is important and constructs the (useful) low-dimensional feature vector. Nonlinear auto-encoders played an important role in auto-associative neural networks [Cottrell and Munro, 1988; Baldi and Hornik, 1988; Bourlard and Kamp, 1988; Oja, 1991]. A special case is the linear auto-encoder in which both the decoder and encoder are linear maps [Oja, 1992]. Perhaps the most famous linear auto-encoder is principal components analysis (PCA), in particular because it is optimal: PCA is the linear auto-encoder that preserves the maximum amount of information (given the dimensionality of the feature space). We study general linear auto-encoders, and enforce sparsity on the encoding linear map on the grounds that a sparse encoder is easier to interpret. A special case of a sparse linear encoder is sparse PCA.

More formally, the data matrix is $X \in \mathbb{R}^{n \times d}$ (each row $x_i \in \mathbb{R}^{1 \times d}$ is a data point in $d$ dimensions). Our
focus is the linear auto-encoder, which, for \( k < d \), is a pair of linear mappings

\[
  h : \mathbb{R}^d \rightarrow \mathbb{R}^k \quad \text{and} \quad g : \mathbb{R}^k \rightarrow \mathbb{R}^d, \]

specified by an encoder matrix \( H \in \mathbb{R}^{d \times k} \) and a decoder matrix \( G \in \mathbb{R}^{k \times d} \). For data point \( x \in \mathbb{R}^d \), the encoded feature is

\[
  z = h(x) = H^T x \in \mathbb{R}^k
\]

and the reconstructed datum is

\[
  \hat{x} = g(z) = G^T z \in \mathbb{R}^d.
\]

Using \( \hat{X} \in \mathbb{R}^{n \times d} \) to denote the reconstructed data matrix, we have

\[
  \hat{X} = XHG.
\]

The pair \((H, G)\) are a good auto-encoder if \( \hat{X} \approx X \), using the squared loss:

**Definition 1 (Information Loss \( \ell(H, X) \)).** The information loss of linear encoder \( H \) is the minimum possible reconstruction error for \( X \) over all linear decoders \( G \):

\[
  \ell(H, X) = \min_{G \in \mathbb{R}^{k \times d}} \| X - XHG \|_F^2 = \| X - XH(XH)^{\dagger} X \|_F^2.
\]

The last formula follows by doing a linear regression to obtain the optimal \( G \).

PCA is perhaps the most famous linear auto-encoder, because it is optimal with respect to information loss. Since \( \operatorname{rank}(XHG) \leq k \), the information loss is bounded by

\[
  \ell(H, X) \geq \| X - X_k \|_F^2,
\]

(for a matrix \( A \), \( A_k \) is its best rank-\( k \) approximation). By the Eckart-Young theorem \( X_k = XV_k V_k^T \), where \( V_k \in \mathbb{R}^{d \times k} \) is the matrix whose columns are the top-\( k \) right singular vectors of \( X \) (see, for example, e-Chapter 9 of Abu-Mostafa et al. [2012]). Thus, the optimal linear encoder is \( H_{opt} = V_k \), with optimal decoder \( G_{opt} = V_k^T \), and, the corresponding top-\( k \) PCA-features are \( Z_{pca} = XV_k \).

Since its early beginnings in Pearson [1901], PCA has become a classic tool for data analysis, visualization and feature extraction. While PCA simplifies the data by concentrating as much information as possible into a few components, those components may not be easy to interpret. In many applications, it is desirable to “explain” the PCA-features using a small number of the original dimensions because the original variables have direct physical significance. For example, in biological applications, they may be genes, or in financial applications they may be assets. One seeks a tradeoff between the fidelity of the features (their ability to reconstruct the data), and the interpretability of the features using a few original variables. We would like the encoder \( H \) to be sparse. Towards this end, we introduce a sparsity parameter \( r \) and require that every column of \( H \) have at most \( r \) non-zero elements. Every feature in an \( r \)-sparse encoding can be “explained” using at most \( r \) original features. Such interpretable factors are known as sparse principal components (SPCA).

We may now formally state the sparse linear encoder problem that we consider in this work:
The lower bound shows that sparsity $r$ loss with respect to PCA, and hence that our algorithm is asymptotically optimal.

Given $X \in \mathbb{R}^{n \times d}$, $\varepsilon > 0$ and $k < \text{rank}(A)$, find, for the smallest possible $r$, an $r$-sparse encoder $H$ for which

$$\ell(H, X) = \|X - XH(XH)^\dagger X\|_F^2 \leq (1 + \varepsilon)\|X - X_k\|_F^2.$$

Note that we seek a relative-error approximation to the optimal loss.

1.1 Notation

Let $\rho = \min\{n, d\} = \text{rank}(X)$ (typically $\rho = d$). We use $A, B, C, \ldots$ for matrices and $a, b, c, \ldots$ for vectors. The standard Euclidean basis vectors are $e_1, e_2, \ldots$ (the dimension will usually be clear from the context).

The singular value decomposition (SVD) allows us to write $X = U \Sigma V^\top$, where the columns of $U \in \mathbb{R}^{n \times \rho}$ are the $\rho$ left singular vectors, the columns of $V \in \mathbb{R}^{d \times \rho}$ are the $\rho$ right singular vectors, and $\Sigma \in \mathbb{R}^{\rho \times \rho}$ is a diagonal matrix of positive singular values $\sigma_1 \geq \cdots \geq \sigma_\rho$. $U$ and $V$ are orthonormal, so $U^\top U = V^\top V = I_\rho$. We give the first polynomial-time algorithm for near-optimal $r$-sparse linear encoder $H$ for which $\|X - XH(XH)^\dagger X\|_F^2 \leq (1 + \varepsilon)\|X - X_k\|_F^2$. Our algorithm constructs an $r$-sparse linear encoder $H$ for which $\|X - XH(XH)^\dagger X\|_F^2 \leq (1 + O(k/\epsilon))\|X - X_k\|_F^2$.

We give the first lower bound on the sparsity $r$ that is required to achieve a $(1 + \epsilon)$-approximation to the information loss of PCA (see Theorem 7).

The lower bound shows that sparsity $r = \Omega(k/\epsilon)$ is required to guarantee $(1 + \epsilon)$-approximate information loss with respect to PCA, and hence that our algorithm is asymptotically optimal.
Iterative Algorithm for Linear Encoder. Our algorithm constructs all $k$ factors simultaneously, in a sense treating all the factors equally. One cannot identify a “top” factor. Most existing sparse PCA algorithms first construct a top sparse PCA factor; then, every next sparse factor must be orthogonal to all previous ones. We develop a similar iterative algorithm by running our “batch” algorithm repeatedly with $k = 1$, each time extracting a provably accurate sparse factor for a residual. We give a performance guarantee for the resulting $k$ factors that are constructed by our algorithm (see Theorem 11). We show that in each step, all factors constructed up to that point are provably accurate. Ours is the first performance guarantee for any iterative scheme of this type, that constructs sparse factors one by one.

Our information loss guarantee for the iterative algorithm is approximately a $(1 + O(\varepsilon \log k))$-factor worse than PCA (up to a small additive error). This bound is not as good as for the batch algorithm, but, in practice, the iterative algorithm is faster, constructs sparser factors and performs well.

Experiments. We show the experimental performance of our algorithms on standard benchmark data sets and compared with some standard benchmark sparse PCA algorithms. The experimental results indicate that our algorithms perform as the theory predicts, and in all cases produces factors which are comparable or better to the standard benchmark algorithms.

1.3 Discussion of Related Work

PCA is the most popular linear auto-encoder, due to its optimality. Nonlinear auto-encoders became prominent with auto-associative neural networks [Cottrell and Munro, 1988; Baldi and Hornik, 1988; Bourlard and Kamp, 1988; Oja, 1991, 1992]. We are unaware of work addressing the more general “sparse linear auto-encoder”.

Sparse Factors. The importance of sparse factors in dimensionality reduction was recognized in some early work: the varimax criterion of Kaiser [1958] was used to rotate the factors and encourage sparsity, and this has been used in multi-dimensional scaling approaches to dimension reduction by Sammon [1969]; Kruskal [1964]. One of the first attempts at sparse PCA used axis rotations and thresholding [Cadima and Jolliffe, 1995]. Since then, sophisticated computational techniques have been developed. In general, these methods address finding just one sparse principal component, and one can apply the algorithm iteratively on the residual after projection to get additional sparse principal components.

Minimizing Information Loss versus Maximizing Variance. The traditional formulation of sparse PCA is as a cardinality constrained variance maximization problem: maximize $v^T A v$ subject to $v^Tv = 1$ and $\|v\|_0 \leq r$, for $A \in \mathbb{R}^{n \times n}$ and $r < n$. A straightforward reduction from MAX-CLIQUE shows this problem to be NP-hard (if $A$ is the adjacency matrix of a graph, then $A$ has a clique of size $k$ if and only if $v^T A v \geq (k - 1)$ for a $k$-sparse unit vector $v$, see Magdon-Ismail [2015]). Sparse PCA is a special case of a generalized eigenvalue problem: maximize $v^T S v$ subject to $v^T Q v = 1$ and $\|v\|_0 \leq r$. This generalized eigenvalue problem is known to be NP-hard [Moghaddam et al., 2008], via a reduction from sparse regression which is NP-hard [Natarajan, 1995; Foster et al., 2014].

This view of PCA as the projection which maximizes variance is due to a historical restriction to symmetric auto-encoders $H^\dagger$ (so $G = H^\dagger$), see for example Oja [1992]. The PCA auto-encoder is symmetric
because $V_k^\dagger = V_k^\top$. Observe that
\[
\text{var}(X) = \|X\|_F^2 = \|X(I - HH^\dagger) + XHH^\dagger\|_F^2 = \|X - XHH^\dagger\|_F^2 + \|XHH^\dagger\|_F^2,
\]
where the last equality is from Pythagoras’ theorem. Minimizing the information loss $\|X - XHH^\dagger\|_F^2$ is equivalent to maximizing $\|XHH^\dagger\|_F^2 = \text{Tr}(H^\dagger X^\top X H)$, the symmetric explained variance. (A similar decomposition holds for the information loss of a general linear auto-encoder and the “true” explained variance). The top-$k$ principal components $V_k$ maximize the symmetric explained variance. This view of PCA as the projection that captures the maximum symmetric explained variance has led to the historical approach to sparse PCA: find a symmetric autoencoder that is sparse and captures the maximum symmetric explained variance. The decomposition of the variance into a sum of information loss and symmetric explained variance means that in an unconstrained setting, minimizing information loss and maximizing the symmetric explained variance are both ways of encouraging $H$ to be close to $V_k$. However, when $H$ is constrained (for example to be sparse), these optimization objectives can produce very different optimal solutions, and there are several reasons to focus on minimizing information loss:

(i) Maximizing variance corresponds to minimizing information loss for symmetric decoders. For the general encoder however, variance has no intrinsic value, but information loss directly captures the unsupervised machine learning goal: the decoder is secondary and what matters is that the encoder produce a compact representation of the data and preserve as much information as possible. Constraints on the decoder (such requiring a symmetric auto-encoder) will translate into a suboptimal encoder that loses more information than is necessary. We are after an encoder into a lower dimensional space that preserves as much information in the data as possible. Hence, to get the most informative sparse features, one should directly minimize the information loss (placing no constraints on the decoder).

(ii) An approximation algorithm for information loss can be converted to an approximation algorithm for variance maximization.

\textbf{Theorem 2.} If $\|X - XHH^\dagger\|_F^2 \leq (1 + \varepsilon) \|X - X_k\|_F^2$, then
\[
\|XHH^\dagger\|_F^2 \geq \|X_k\|_F^2 - \varepsilon \|X - X_k\|_F^2 \geq \left(1 - \frac{\rho - k}{k}\varepsilon\right)\|X_k\|_F^2.
\]

\textbf{Proof.} Since $\|X - XHH^\dagger\|_F^2 = \|X\|_F^2 - \|XHH^\dagger\|_F^2 \leq (1 + \varepsilon) \|X - X_k\|_F^2$, we have
\[
\|XHH^\dagger\|_F^2 \geq \|X\|_F^2 - (1 + \varepsilon) \|X - X_k\|_F^2 = \|X_k\|_F^2 - \varepsilon \|X - X_k\|_F^2.
\]
The second inequality follows from the bound $\|X - X_k\|_F^2 \leq \|X_k\|_F^2 \cdot (\rho - k)/k$. \hfill \square

Thus, a relative error approximation for reconstruction error gives a relative error approximation for explained variance. However, a decoder which gives a relative error approximation for symmetric explained variance does not immediately give a relative error approximation for information loss.

(iii) Explained variance is not well defined for general encoders, whereas information loss is well defined. As Zou et al. (2006) points out, one has to be careful when defining the explained variance for general encoders. The interpretation of $\text{Tr}(H^\dagger X^\top X H)$ as an explained variance relies on two important
properties: the columns in $H$ are orthonormal ("independent") directions and they are decorrelated from each other, that is $H^T H = I_k$ and $H^T X^T X H$ is diagonal. The right singular vectors are the unique factors having these two properties. Therefore, when one introduces a cardinality constraint, one has to give up one or both of these properties, and typically one relaxes the decorrelation requirement. Now, as Zou et al. [2006] points out, when factors are correlated, the variance is not straightforward to define, and $\text{Tr}(H^T X^T X H)$ is an optimistic estimate of explained variance. Zou et al. [2006] computes a “variance after decorrelation” to quantify the quality of sparse PCA. Their solution is not completely satisfactory since the order in which factors are sequentially decorrelated can change the explained variance. Our solution is simple: use the information loss which is not only the natural metric one is interested in, but is always well defined.

Heuristics for Sparse PCA via Maximizing Variance. Despite the complications with with interpreting the explained variance with general encoders which produce correlated factors, all the heuristics we are aware of has focused on maximizing the variance. With a sparsity constraint, the problem becomes combinatorial and the exhaustive algorithm requires $O(d r^2 (\frac{d}{r}))$ computation. This exponential running time can be improved to $O(d^{r+1})$ for a rank-$r$ perturbation of the identity. None of these exhaustive algorithms are practical for high-dimensional data. Several heuristics exist. Trendafilov et al. [2003] and Zou et al. [2006] take an $L_1$ penalization view. DSPCA (direct sparse PCA) d’Aspremont et al. [2007] also uses an $L_1$ sparsifier but solves a relaxed convex semidefinite program which is further refined in d’Aspremont et al. [2008] where they also tractable sufficient condition for testing optimality. The simplest algorithms use greedy forward and backward subset selection. For example, Moghaddam et al. [2006] develop a greedy branch and bound algorithm based on spectral bounds with $O(d^3)$ running time for forward selection and $O(d^3)$ running time for backward selection. An alternative view of the problem is as a sparse matrix reconstruction problem; for example Shen and Huang [2008] obtain sparse principal components using regularized low-rank matrix approximation.

Theoretical guarantees. The heuristics are quite mature, but few theoretical guarantees are known. We are not aware of any polynomial time algorithms with guarantees on optimality. In Asteris et al. [2014], the sparse PCA problem is considered with an additional non-negativity constraint; and the authors give an algorithm which takes as input a parameter $k$, has running time $O(d^{k+1} \log d + d^k r^3)$ and constructs a sparse solution that is a $(1 - \frac{1}{r})\|S - S_k\|_2/\|S\|_2)$-factor from optimal. The running time is not practical when $k$ is large and the approximation guarantee is only non-trivial when the spectrum of $S$ is rapidly decaying. Further, the approximation guarantee only applies to constructing the first sparse PCA and it is not clear how this result can be extended if the algorithm is applied iteratively.

To our knowledge, there are no known guarantees for top-$k$ sparse factors with respect to PCA. Within the more general setting of sparse linear auto-encoders, we solve two open problems: (i) We determine the best approximation guarantee with respect to the optimal linear encoder (PCA) that can be achieved using a linear encoder with sparsity $r$; (ii) We give low order polynomial algorithms that achieve an approximation guarantee with respect to PCA using a sparsity that is within a factor of two of the minimum required sparsity. Our algorithms apply to constructing $k$ sparse linear features with performance comparable to top-$k$ PCA.
2 Optimal Sparse Linear Encoder

We show a black-box reduction of sparse linear encoding to column subset selection, and so it is worthwhile to first discuss background in column subset selection. We then use column subset selection algorithms to construct provably accurate sparse auto-encoders. Finally, we modify our main algorithm so that it can select features iteratively and prove a bound for this iterative setting.

2.1 Column Subset Selection Problem (CSSP)

For \( X = [f_1, \ldots, f_d] \), we let \( C = [f_{i_1}, f_{i_2}, \ldots, f_{i_r}] \) denote a matrix formed using \( r \) columns “sampled” from \( X \), where \( 1 \leq i_1 < i_2 < \cdots < i_r \leq d \) are distinct column indices. Column sampling is a linear operation, and we can use a matrix \( \Omega \in \mathbb{R}^{d \times r} \) to perform the column sampling, \[ C = X \Omega, \quad \text{where} \quad \Omega = [e_{i_1}, e_{i_2}, \ldots, e_{i_r}], \]
and \( e_i \) are the standard basis vectors in \( \mathbb{R}^d \) (post-multiplying \( X \) by \( e_i \) “samples” the \( i \)th column of \( X \)). The columns of \( C \) span a subspace in the range of \( X \) (which is the span of the columns of \( X \)). Any column sampling matrix can be used to construct an \( r \)-sparse matrix.

Lemma 3. Let \( \Omega = [e_{i_1}, e_{i_2}, \ldots, e_{i_r}] \in \mathbb{R}^{d \times r} \) and let \( A \in \mathbb{R}^{r \times k} \) be any matrix. Then \( \Omega A \in \mathbb{R}^{d \times k} \) is \( r \)-sparse, i.e., each column of \( \Omega A \) has at most \( r \) non-zero entries.

Proof. Let \( A = [a_1, \ldots, a_k] \) and consider \( \Omega a_j \) which is column \( j \) of \( \Omega A \). A zero-row of \( \Omega \) results in the corresponding entry in \( \Omega a_j \) being zero. Since \( \Omega \) has \( r \) non-zero rows, there are at most \( r \) non-zero entries in \( \Omega a_j \).

Given columns \( C \), we define \( X_C = C^\dagger X \) to be the matrix obtained by projecting all the columns of \( X \) onto the subspace spanned by \( C \). For any matrix \( \hat{X} \) whose columns are in the span of \( C \), \( \| X - X_C \|_F^2 \leq \| X - \hat{X} \|_F^2 \). Let \( X_{C,k} \in \mathbb{R}^{n \times d} \) be the optimal rank-\( k \) approximation to \( X_C \) obtained via the SVD of \( X_C \).

Lemma 4 (See, for example, Boutsidis et al. [2014]). \( X_{C,k} \) is a rank-\( k \) matrix whose columns are in the span of \( C \). Let \( \hat{X} \) be any rank-\( k \) matrix whose columns are in the span of \( C \). Then, \( \| X - X_{C,k} \|_F^2 \leq \| X - \hat{X} \|_F^2 \).

That is, \( X_{C,k} \) is the best rank-\( k \) approximation to \( X \) whose columns are in the span of \( C \). An efficient algorithm to compute \( X_{C,k} \) is also given in Boutsidis et al. [2014]. The algorithm runs in \( O(nrd + (n + d)r^2) \) time. We reproduce that algorithm here.

| Algorithm to compute \( X_{C,k} \) |
|----------------------------------|
| **Inputs:** \( X \in \mathbb{R}^{n \times d} \), \( C \in \mathbb{R}^{n \times r} \), \( k \leq r \). |
| **Output:** \( X_{C,k} \in \mathbb{R}^{n \times d} \). |
| 1: Compute a QR-factorization of \( C \) as \( C = QR \), with \( Q \in \mathbb{R}^{n \times r} \), \( R \in \mathbb{R}^{r \times r} \). |
| 2: Compute \( (Q^\dagger X)_k \in \mathbb{R}^{r \times d} \) via SVD (the best rank-\( k \) approximation to \( Q^\dagger X \)). |
| 3: Return \( X_{C,k} = Q(Q^\dagger X)_k \in \mathbb{R}^{n \times d} \). |

We mention that it is possible to compute a \((1 + \epsilon)\)-approximation to \( X_{C,k} \) more quickly using randomized projections [Boutsidis and Woodruff, section 3.5.2].
2.2 Sparse Linear Encoders from CSSP

The main result of this section is to show that if we can obtain a set of columns \( C \) for which \( X_{C,k} \) is a good approximation to \( X \), then we can get a good sparse linear encoder for \( X \). We first give the algorithm for obtaining an \( r \)-sparse linear encoder from \( r \)-columns \( C \), and then we give the approximation guarantee. For simplicity, in the algorithm below we assume that \( C \) has full column rank. This is not essential, and if \( C \) is rank deficient, then the algorithm can be modified to first remove the dependent columns in \( C \).

**Blackbox algorithm to compute encoder from CSSP**

| Inputs: \( X \in \mathbb{R}^{n \times d}; C \in \mathbb{R}^{n \times r} \) with \( C = X \Omega \) and \( \Omega = [e_1, \ldots, e_n] \); \( k \leq r \). |
|---|
| Output: \( r \)-sparse linear encoder \( H \in \mathbb{R}^{d \times k} \). |
| 1: Compute a QR-factorization of \( C \) as \( C = QR \), with \( Q \in \mathbb{R}^{n \times r} \), \( R \in \mathbb{R}^{r \times r} \). |
| 2: Compute the SVD of \( R^{-1}(Q^T X)_k \), \( R^{-1}(Q^T X)_k = U_R \Sigma_R V_R^T \), where \( U_R \in \mathbb{R}^{r \times k} \), \( \Sigma_R \in \mathbb{R}^{k \times k} \) and \( V_R \in \mathbb{R}^{d \times k} \). |
| 3: Return \( H = \Omega U_R \in \mathbb{R}^{d \times k} \). |

In the algorithm above, since \( C \) has full column rank, \( R \) is invertible. Note that the algorithm can be modified to accommodate \( r < k \), in which case it will output fewer than \( k \) factors in the output encoding. In step 2, even though \( R^{-1}(Q^T X)_k \) is an \( r \times d \) matrix, it has rank \( k \), hence the dimensions of \( U_R, \Sigma_R, V_R \) depend on \( k \), not \( r \). By Lemma 3, the encoder \( H \) produced by the algorithm is \( r \)-sparse. Also observe that \( H \) has orthonormal columns, as is typically desired for an encoder:

\[
H^T H = U_R^T \Omega^T \Omega U_R = U_R^T U_R = I_k.
\]

Actually, the encoder \( H \) has a much stronger property than \( r \)-sparsity, namely that in every column the nonzeros can only be located at the same \( r \) coordinates. We now compute the running time of the algorithm. The first two steps are as in the algorithm to compute \( X_{C,k} \) and so take \( O(ndr + (n + d)r^2) \) time (the multiplication by \( R^{-1} \) and the computation of an additional SVD do not affect the asymptotic running time). The last step involves two matrix multiplications which can be done in \( O(r^2 k + drk) \) additional time, which also does not affect the asymptotic running time of \( O(ndr + (n + d)r^2) \). We now show that the encoder \( H \) produced by the algorithm is good if the columns result in a good rank-\( k \) approximation \( X_{C,k} \).

**Theorem 5** (Blackbox encoder from CSSP). Given \( X \in \mathbb{R}^{n \times d} \), \( C = X \Omega \in \mathbb{R}^{n \times r} \) with \( \Omega = [e_1, \ldots, e_n] \) and \( k \leq r \), let \( H \) be the \( r \)-sparse linear encoder produced by the algorithm above, which runs in \( O(ndr + (n + d)r^2) \) time. Then, the information loss satisfies

\[
\ell(H, X) = \|X - XH(H)^T X\|_F^2 \leq \|X - X_{C,k}\|_F^2.
\]

The theorem says that if we can find a set of \( r \) columns within which a good rank-\( k \) approximation to \( X \) exists, then we can construct a good linear sparse encoder.

**Proof.** We show that there is a decoder \( G \) for which \( \|X - XHG\|_F^2 = \|X - X_{C,k}\|_F^2 \). The theorem then follows because the optimal decoder cannot have higher reconstruction error. We use \( U_R, \Sigma_R \) and \( V_R \) as defined in
the algorithm, and set \( G = \Sigma_R V_R^T \). We then have,

\[
XHG = X\Omega U_R \Sigma_R V_R^T = X \Sigma_R V_R^T R^{-1} Q^t X_k = CR^{-1} Q^t X_k
\]

The first step is by construction in the algorithm because \( U_R, \Sigma_R, V_R \) is obtained from the SVD of \( R^{-1} (Q^t X)_k \). The second step is because \( C = X\Omega \). Since \( C = QR \) (and \( R \) is invertible), it follows that \( CR^{-1} = Q \). Hence,

\[
XHG = Q (Q^t X)_k = X_{C,k},
\]

hence \( \|X - XHG\|_F^2 = \|X - X_{C,k}\|_F^2 \), concluding the proof.

What remains is to find a sampling matrix \( \Omega \) which gives a good set of columns \( C = X\Omega \) for which \( \|X - X_{C,k}\|_F^2 \) is small. The main tool to obtain \( C \) and \( \Omega \) was developed in Boutsidis et al. [2014] which gave a constant factor deterministic approximation algorithm and a relative-error randomized approximation algorithm. We state a simplified form of the result and then discuss various ways in which this result can be enhanced. The main point is that any algorithm to construct a good set of columns can be used as a black box to get a sparse linear encoder.

**Theorem 6** (Near-optimal CSSP [Boutsidis et al., 2014]). Given \( X \in \mathbb{R}^{n \times d} \) of rank \( \rho \) and target rank \( k \):

(i) (Theorem 2 in Boutsidis et al. [2014]) For sparsity parameter \( r > k \), there is a deterministic algorithm which runs in time \( T_{V_k} + O(ndk + dk^3) \) to construct a sampling matrix \( \Omega = [e_{i_1}, \ldots, e_{i_r}] \) and corresponding columns \( C = X\Omega \) such that

\[
\|X - X_{C,k}\|_F^2 \leq \left( 1 + \frac{1}{(1 - \sqrt{r/k})^2} \right) \|X - X_k\|_F^2.
\]

(ii) (Simplified Theorem 5 in Boutsidis et al. [2014]) For sparsity parameter \( r > 5k \), there is a randomized algorithm which runs in time \( O(ndk + dk^3) \) to construct a sampling matrix \( \Omega = [e_{i_1}, \ldots, e_{i_r}] \) and corresponding columns \( C = X\Omega \) such that

\[
\mathbb{E} \left[ \|X - X_{C,k}\|_F^2 \right] \leq \left( 1 + \frac{5k}{r - 5k} \right) \|X - X_k\|_F^2.
\]

**Proof.** (Sketch for part (ii).) We follow the proof in Boutsidis et al. [2014], using the same notation in Boutsidis et al. [2014]. Choose \( 5k \) columns for the initial constant factor approximation and set the accuracy \( \varepsilon_0 \) for the approximate SVD to compute \( \hat{V}_k \) to a constant so that \( \varepsilon_0 = (1 + \varepsilon_0)(1 + (1 - \sqrt{5/17})^{-2}) = 5 \). The adaptive sampling step ensures a \( (1 + c_0 k/s) \)-approximation for the reconstruction, where \( s = r - 5k \).

**Comments.**

1. In part (ii) of the theorem, setting \( r = 5k + 5k/\varepsilon = O(k/\varepsilon) \) ensures that \( X_{C,k} \) is a \( (1 + \varepsilon) \)-reconstruction of \( X_k \) (in expectation). At the expense of an increase in the running time the sparsity can be reduced to \( r \approx 2k/\varepsilon \) while still giving a \( (1 + \varepsilon) \)-reconstruction. The message is that \( O(k/\varepsilon) \)-sparsity suffices to get a \( (1 + \varepsilon) \)-accurate reconstruction.
2. Part (ii) of the theorem gives a bound on $|X - X_{C,k}|^2_F$. The expectation is with respect to random choices in the algorithm. Using an application of Markov’s inequality to the positive random variable $|X - X_{C,k}|^2_F - |X - X_k|^2_F$, $|X - X_{C,k}|^2_F \leq (1 + 2\varepsilon)||X - X_k||^2_F$ holds with probability at least $\frac{1}{2}$. This can be boosted to high-probability, at least $1 - \delta$, for an additional $\log \frac{1}{\delta}$ factor increase in the running time.

3. In part (i) of the theorem $V_k$ (the top-$k$ right singular vectors) are used in the algorithm, and $T_{V_k}$ is the time to compute $V_k$. To compute $V_k$ exactly, the only known algorithm is via the full SVD of $X$, which takes $O(nd\min\{n, d\})$ time. It turns out that an approximate SVD will do. Suppose that $\hat{V}_k$ satisfies

$$\|X - X\hat{V}_k\hat{V}_k^T\|_F^2 \leq \alpha\|X - X_k\|_F^2.$$ 

The approximation $\hat{V}_k$ can be used in the algorithm instead of $V_k$ and the error will increase by an additional factor of $\alpha$. Boutsidis et al. [2014] gives an efficient randomized approximation for $V_k$ and there is also a recent deterministic algorithm given in Ghashami and Phillips [2013, Theorem 3.1] which computes such an approximate $\hat{V}_k$ in time $O(ndk\varepsilon^{-2})$ with $\alpha = 1 + \varepsilon$.

4. The details of the algorithm that achieves part (ii) of the theorem are given in Boutsidis et al. [2014]. We simply state the three main steps.

   (i) Use a randomized projection to compute an approximation $\hat{V}_k$.
   (ii) Apply the algorithm from part (i) of the theorem using $\hat{V}_k$ to get a constant factor approximation.
   (iii) Apply one round of randomized adaptive column sampling, Deshpande and Vempala [2006] which boosts the constant factor approximation to a $1 + \varepsilon$ approximation.

This entire algorithm can be de-randomized to give a deterministic algorithm by using the deterministic approximation for $\hat{V}_k$ from Ghashami and Phillips [2013] and a derandomization of the adaptive sampling step which appeared in a recent result Boutsidis and Woodruff [2014]. The tradeoff will be a non-trivial increase in the running time. The entire algorithm can also be made to run in input-sparsity-time (see Boutsidis and Woodruff for details).

5. **Doubly sparse auto-encoders.** It is possible to construct an $O(k/\varepsilon)$-sparse linear auto-encoder and a corresponding “sparse” decoder with the following property: the reconstruction $XHG$ has rows which are all linear combinations of $O(k/\varepsilon)$ rows of $X$. Thus, the encoding identifies features which have loadings on only a few dimensions, and the decoder for the encoding is based on a small number of data points. Further, the reconstruction error is near optimal, $\|X - XHG\|_F^2 \leq (1 + \varepsilon)\|X - X_k\|_F^2$.

We give the rough sketch for this doubly sparse linear auto-encoder, without getting into too many details. The main tool is the CΦR matrix decomposition Drineas and Kannan [2003]. An asymptotically optimal construction was given in Boutsidis and Woodruff [2014] which constructs columns $C = X\Omega_1 \in \mathbb{R}^{n \times r_1}$ and rows $R = \Omega_2^T X \in \mathbb{R}^{r_2 \times d}$ and a rank-$k$ matrix $\Phi \in \mathbb{R}^{r_1 \times r_2}$ for which $\|X - C\Phi R\|_F^2 \leq (1 + \varepsilon)\|X - X_k\|_F^2$, where $\Omega_1 = [e_{i_1}, \ldots, e_{i_{r_1}}]$ and $\Omega_2 = [e_{i_{r_1}} \ldots, e_{i_{r_2}}]$ are sampling matrices with $r_1 = O(k/\varepsilon)$ and $r_2 = O(k/\varepsilon)$. Let $\Phi = U_\Phi \Sigma_\Phi V_\Phi^T$ be the SVD of $\Phi$, where $U_\Phi \in \mathbb{R}^{r_1 \times k}$, $\Sigma_\Phi \in \mathbb{R}^{k \times k}$, $V_\Phi \in \mathbb{R}^{r_2 \times k}$. Then, we set the encoder to $H = \Omega_1 U_\Phi$ which is $O(k/\varepsilon)$-sparse, and the decoder to $G = \Sigma_\Phi V_\Phi^T \Omega_2^T X$. The reconstruction is $X\Omega_1 U_\Phi \Sigma_\Phi V_\Phi^T \Omega_2^T X$; The matrix $\Omega_2^T X$ contains $O(k/\varepsilon)$ rows of $X$ and so the reconstruction is based on linear combinations of these rows.

The trade off for getting this doubly-sparse encoding is a decrease in the accuracy, since the decoder is now only getting an approximation to the best rank-$k$ reconstruction within the column-span of $C$. The
advantage of the doubly sparse encoder is that it identifies a small set of $O(k/\varepsilon)$ original features that are important for the dimension-reduced features. It also simultaneously identifies a small number of $O(k/\varepsilon)$ data points that are important for reconstructing the entire data matrix.

We are now ready for the main theoretical result of the section. By using Theorem 6 in our black-box linear encoder, we obtain our algorithm to construct a sparse linear encoder with a provable approximation guarantee.

### Sparse Linear Encoder Algorithm

**Inputs:** $X \in \mathbb{R}^{n \times d}$; target rank $k \leq \text{rank}(X)$; sparsity $r > k$.

**Output:** Near-optimal $r$-sparse linear encoder $H \in \mathbb{R}^{d \times k}$.

1. Use the algorithm from Theorem 6-(ii) to compute columns $C = X\Omega \in \mathbb{R}^{n \times r}$, with inputs $X$, $k$, $r$.
2. Return the encoder $H$ computed by using $X$, $C$, $k$ as input to the CSSP-blackbox encoder algorithm.

Using Theorem 6 in Theorem 5, we have an approximation guarantee for our algorithm.

**Theorem 7 (Sparse Linear Encoder).** Given $X \in \mathbb{R}^{n \times d}$ of rank $\rho$, the target number of sparse PCA vectors $k \leq \rho$, and sparsity parameter $r > 5k$, there is a randomized algorithm running in time $O(ndr + (n + d)r^2 + dk^3)$ which constructs an $r$-sparse encoder $H$ such that:

$$E[\ell(H, X) = E[\|X - XH(XH)^\dagger X\|_F^2] \leq \left(1 + \frac{5k}{r - 5k}\right)\|X - X_k\|_F^2.$$  

**Comments.**

1. The expectation is over the random choices made in the algorithm to construct $H$. All the comments from Theorem 5 apply here as well. In particular, this result is easily converted to a high probability guarantee, or even a deterministic guarantee at the expense of some accuracy and a (polynomial in $d$, $r$)-factor increase in the computational cost.

2. The guarantee is with respect to $\|X - X_k\|_F^2$, which is the best possible rank-$k$ reconstruction with $k$ dense optimal features obtained from PCA. Our result shows that $O(k/\varepsilon)$-sparse features suffices to mimic top-$k$ (dense) PCA within a $(1 + \varepsilon)$-factor error.

   We presented the simplified version of the results requiring sparsity $r > 5k$. Actually our technique can be applied for any choice of $r > k$ with approximation guarantee $c(1 + 1/(1 - \sqrt{k/r})^2)$ where $c \approx 1$ is a constant.

3. The reconstruction error using our $r$-sparse encoder is compared with PCA, not with the optimal $r$-sparse encoder. With respect to the optimal $r$-sparse encoder, our approximation could be much better. It would be a challenging task to get an approximation guarantee with respect to the best possible $r$-sparse linear-encoder.

### 2.3 Lower Bound on Sparsity

We define the combined sparsity of $H$ to be the number of its rows that are non-zero. When $k=1$, the combined sparsity equals the sparsity of the single factor. The combined sparsity is the total number of dimensions.
which have non-zero loadings among all the factors. Our algorithm produces an encoder with combined sparsity $O(k/\varepsilon)$ and comes within $(1 + \varepsilon)$ of the minimum possible information loss. We show that this is worst case optimal. Specifically, there is a matrix $X$ for which any linear encoder which can achieve a $(1 + \varepsilon)$-approximate reconstruction error as compared to PCA must have a combined sparsity $r \geq k/\varepsilon$. So $\Omega(k/\varepsilon)$-sparsity is required to achieve a $(1 + \varepsilon)$-approximation. The common case that is studied in the literature is with $k = 1$ (constructing a sparse top principal component). Our lower bound shows that $\Omega(1/\varepsilon)$-sparsity is required to get a $(1 + \varepsilon)$-approximation and our algorithm asymptotically achieves this lower bound, therefore we are asymptotically optimal.

We show the converse of Theorem 5, namely that from a linear auto-encoder with combined sparsity $r$, we can construct $r$ columns $C$ for which $X_{C,k}$ is a good approximation to $X$. We then use the lower bound proved in Boutsidis et al. 2014, Section 9.2 which states that for any $\delta > 0$, there is a matrix $B$ such that for any set of $r$ of its columns $C$,

\[
\|B - B_{C,k}\|_F^2 \geq \|B - CC^\dagger B\|_F^2 \geq \left(1 + \frac{k}{r} - \delta\right)\|B - B_k\|_F^2. \tag{1}
\]

Now suppose that $H$ is a linear encoder with combined sparsity $r$ for this matrix $B$ from Boutsidis et al. 2014, Section 9.2, and let $G$ be a decoder satisfying

\[
\|B - BHG\|_F^2 \leq (1 + \varepsilon)\|B - B_k\|_F^2.
\]

We offer the following elementary lemma which allows one to construct columns from a sparse encoder.

**Lemma 8.** Suppose $H$ is a linear encoder for $B$ with combined sparsity $r$ and with decoder $G$. Then, $BH G = CY$ for some set of $r$ columns of $B$, denoted $C$, and some matrix $Y \in \mathbb{R}^{r \times d}$.

**Proof.** Let $1 \leq i_1 < i_2 \cdots < i_r \leq d$ be the indices of the non-zero rows of $H$ and let $\Omega = \{e_{i_1}, \ldots, e_{i_r}\}$ be a sampling matrix for $B$. Every column of $H$ is in the subspace spanned by the columns in $\Omega$. Hence, the projection of $H$ onto the columns in $\Omega$ gives back $H$, that is $H = \Omega \Omega^\dagger H$. So, $BH G = B \Omega \Omega^\dagger H = CY$, where $C = \Omega \Omega^\dagger H$.

By Lemma 8 and because $\|B - CC^\dagger B\|_F^2 \leq \|B - CY\|_F^2$ for any $Y$, we have:

\[
\|B - CC^\dagger B\|_F^2 \leq \|B - CY\|_F^2 = \|B - BHG\|_F^2 \leq (1 + \varepsilon)\|B - B_k\|_F^2. \tag{2}
\]

It follows from eq:lower1 and eq:lower2 that $\varepsilon \geq k/r$. Our algorithm gives a reconstruction error $\varepsilon = O(k/r)$, and so our algorithm is asymptotically worst-case optimal. The conclusion is that no linear encoder with combined sparsity $r$ can achieve an approximation ratio which is smaller than $(1 + k/r)$.

**Theorem 9 (Lower Bound on Sparsity).** There exists a data matrix $X$ for which every $r$-sparse encoder with $r < k/\varepsilon$ has an information loss which is strictly greater than $(1 + \varepsilon)\|X - X_k\|_F^2$.

This theorem holds for general linear auto-encoders, and so the lower bound also applies to the symmetric auto-encoder $HH^\dagger$, the traditional formulation of sparse PCA. For the case $k = 1$, any $r$-sparse unit norm $v$, $\|B - Bv v^\dagger\|_F^2 \geq \left(1 + \frac{1}{r}\right)\|B - B_1\|_F^2$, or the explained variance (the variance in the residual) is $v^\dagger B^\dagger Bv$ which is upper-bounded by

\[
v^\dagger B^\dagger Bv \leq \|B_1\|_F^2 - \frac{1}{r} \|B - B_1\|_F^2.
\]
Our algorithm achieves an explained variance which is \( \|B_1\|_F^2 - \Omega(\frac{1}{d}) \|B - B_1\|_F^2 \). Note that with respect to explained variance, the input matrix \( A = [1, 1, \ldots, 1] \) immediately gives an upper bound on the approximation ratio of \( (1 - r/d) \) for the top \( r \)-sparse PCA, since every subset of \( r \) columns of \( A \) has spectral norm \( r \) whereas the spectral norm of \( A \) is \( d \).

### 2.4 Iterative Sparse Linear Encoders

Our previous result is strong in the sense that every vector (column) in the linear encoder is \( r \)-sparse with non-zero loadings on the same set of \( r \) original feature dimensions. From our lower bound, we know that the combined sparsity of \( H \) must be at least \( k/\epsilon \) to achieve reconstruction error \( (1+\epsilon)\|X - X_k\|_2 \) (in the worst case), so our algorithm from Section 2.2 is optimal in that sense. The algorithm is a “batch” algorithm in the sense that, given \( k \), it constructs all the \( k \) factors in \( H \) simultaneously. We will refer to this algorithm as the “batch algorithm”. The batch algorithm may have non-zero loadings on all the \( r \) non-zero rows for every feature vector (column \( h_i \) of \( H \)). Further, the batch algorithm does not distinguish between the \( k \)-factors. That is, there is no top component, second component, and so on.

The traditional techniques for sparse PCA construct the factors iteratively. We can run our batch algorithm in an iterative mode, where in each step we set \( k = 1 \) and compute a sparse factor for a residual matrix. By constructing our \( k \) features iteratively (and adaptively), we identify an ordering among the \( k \) features. Further, we might be able to get each feature sparser while still maintaining a bound on the combined sparsity. The problem is that a straightforward reduction of the iterative algorithm to CSSP is not possible. So we need to develop a new iterative version of the algorithm for which we can prove an approximation guarantee. The iterative algorithm constructs each factor in the encoder sequentially, based on the residual from the reconstruction using the previously constructed factors. One advantage of the iterative algorithm is that it can control the sparsity of each factor independently to achieve the desired approximation bound. Recall that the encoder \( H = [h_1, \ldots, h_k] \) is \((r_1, \ldots, r_k)\)-sparse if \( \|h_i\|_0 \leq r_i \). The iterative algorithm is summarized below.

| Iterative Sparse Linear Encoder Algorithm |
|------------------------------------------|
| **Inputs:** \( X \in \mathbb{R}^{n \times d} \); target rank \( k \leq \text{rank}(X) \); sparsity parameters \( r_1, \ldots, r_k \). |
| **Output:** \((r_1, \ldots, r_k)\)-sparse linear encoder |
| 1. Set the residual \( \Delta = X \) and \( H = [\]. |
| 2. for \( i = 1 \) to \( k \) do |
| 3. Compute an encoder \( h \) for \( \Delta \) using the batch algorithm with \( k = 1 \) and sparsity parameter \( r = r_i \). |
| 4. Update the encoder by adding \( h \) to it: \( H \leftarrow [H, h] \). |
| 5. Update the residual \( \Delta \): \( \Delta \leftarrow X - \text{XH}(\text{XH})^\dagger X \). |
| 6. end for |
| 7. Return the \((r_1, \ldots, r_k)\)-sparse encoder \( H \in \mathbb{R}^{n \times k} \). |

The main iterative step in the algorithm is occurring in steps 3,4 above where we augment \( H \) by computing a top sparse encoder for the residual obtained from the current \( H \). The next lemma bounds the reconstruction error for this iterative step in the algorithm.
Lemma 10. Suppose, for $k \geq 1$, $H_k = [h_1, \ldots, h_k]$ is an encoder for $X$, satisfying

$$
\|X - XH_k(XH_k)^\dagger X\|^2_F = \text{err}.
$$

Given a sparsity $r > 5$, one can compute in time $O(ndr + (n + d)r^2)$ an $r$-sparse feature vector $h_{k+1}$ such that for the encoder $H_{k+1} = [h_1, \ldots, h_k, h_{k+1}]$, the reconstruction error satisfies

$$
\mathbb{E}\left[\|X - XH_{k+1}(XH_{k+1})^\dagger X\|^2_F\right] = (1 + \delta)(\text{err} - \|X - XH_k(XH_k)^\dagger X\|^2_F),
$$

where $\delta \leq 5/(r - 5)$.

Proof. Let $G_k = (XH_k)^\dagger X$ and $B = X - XH_kG_k$. We have that $\|B\|^2_F = \text{err}$. Run our batch algorithm from Theorem 7 on $B$ with $k = 1$ and sparsity parameter $r$ to obtain an $r$-sparse encoder $h_{k+1}$ and corresponding decoder $g_{k+1}$ satisfying

$$
\mathbb{E}\left[\|B - Bh_{k+1}g_{k+1}\|^2_F\right] = (1 + \delta)\|B - B_1\|^2_F,
$$

with $\delta \leq 5/(r - 5)$. Now, the RHS is $\|B - B_1\|^2_F = \|B\|^2_F - \|B_1\|^2_F = \text{err} - \|B\|^2_F$. The LHS is

$$
\mathbb{E}\left[\|B - Bh_{k+1}g_{k+1}\|^2_F\right] = \mathbb{E}\left[\|X - XH_kG_k - Xh_{k+1}g_{k+1}^T + XH_kG_kh_{k+1}g_{k+1}^T\|^2_F\right]
$$

$$
= \mathbb{E}\left[\|X - XH_k(G_k - G_kh_{k+1}g_{k+1}^T) - Xh_{k+1}g_{k+1}^T\|^2_F\right]
$$

$$
= \mathbb{E}\left[\|X - XH_{k+1}G_{k+1}\|^2_F\right],
$$

where $G_{k+1} = [G_k - g_{k+1}h_{k+1}^T G_k, g_{k+1}]$. That is, $H_{k+1}$ with the decoder $G_{k+1}$ satisfies the expected error bound in the lemma, so the optimal decoder cannot do worse in expectation. \qed

We note that the iterative algorithm produces an encoder $H$ which is not guaranteed to be orthonormal. This is not critical for us, since the information loss of the encoder is based on the minimum possible reconstruction error, and we can compute this information loss even if the encoder is not orthonormal. Observe also that, if so desired, it is possible to orthonormalize the columns of $H$ without changing the combined sparsity.

Lemma 10 gives a bound on the reconstruction error for an iterative addition of the next sparse encoder vector. As an example of how we apply Lemma 10, suppose the target rank is $k = 2$. We start by constructing $h_1$ with sparsity $r_1 = 5 + 5/\varepsilon$, which gives us $(1 + \varepsilon)\|X - X_1\|^2_F$ reconstruction error. We now construct $h_2$, also with sparsity $r_2 = 5 + 5/\varepsilon$. The final reconstruction error for $H = [h_1, h_2]$ is bounded by

$$
\|X - XH(XH)^\dagger X\|^2_F \leq (1 + \varepsilon)^2\|X - X_2\|^2_F + \varepsilon(1 + \varepsilon)\|X - X_1\|^2_F.
$$

On the other hand, our batch algorithm uses sparsity $r = 10 + 10/\varepsilon$ in each encoder $h_1, h_2$ and achieves reconstruction error $(1 + \varepsilon)^2\|X - X_2\|^2_F$. The iterative algorithm uses sparser features, but pays for it a little in reconstruction error. The additive term is small: it is $O(\varepsilon)$ and depends on $\|X - X_1\|^2_F = \sigma_2^2$, which in practice is smaller than $\|X - X_2\|^2_F = \sigma_3^2 + \cdots + \sigma_d^2$. In practice, though the theoretical bound for the iterative algorithm is slightly worse than the batch algorithm guarantee, the iterative algorithm performs comparably to the batch algorithm, it is more flexible and able to generate encoder vectors that are sparser than the batch algorithm.

Using the iterative algorithm, we can tailor the sparsity of each encoder vector separately to achieve a
desired accuracy. It is algebraically intense to prove a bound for a general choice of the sparsity parameters \( r_1, \ldots, r_k \), so, for simplicity, we prove a bound for a specific choice of the sparsity parameters which slowly increase for each additional encoder vector. We get the following result.

**Theorem 11** (Adaptive iterative encoder). Given \( X \in \mathbb{R}^{n \times d} \) of rank \( \rho \) and \( k < \rho \), there is an algorithm to compute encoder vectors \( h_1, h_2, \ldots, h_k \) iteratively with each encoder vector \( h_j \) having sparsity \( r_j = 5 + \lceil 5j/\varepsilon \rceil \) such that for every \( \ell = 1, \ldots, k \), the encoder \( H_\ell := [h_1, h_2, \ldots, h_\ell] \) has information loss:

\[
E \left[ \|X - X H_\ell (X H_\ell)^\dagger X\|_F^2 \right] \leq (\ell \varepsilon)^3 \|X - X_\ell\|_F^2 + \varepsilon \ell + \varepsilon^2 \|X - X_1\|_F^2. \tag{3}
\]

The running time to compute all the encoder vectors is \( O(ndk^2 \varepsilon^{-1} + (n + d)k^3 \varepsilon^{-2}) \).

**Comments.**

1. \((\ell \varepsilon)^3\) is a very slowly growing in \( \ell \). For example, for \( \varepsilon = 0.01 \) and \( \ell = 100 \), \( \varepsilon \ell \approx 1.04 \). Asymptotically, \((\ell \varepsilon)^3 = 1 + O(\varepsilon \log \ell)\), so up to a small additive term, we have a relative error approximation. The message is that we get a reasonable approximation guarantee for our iterative algorithm, where no such bounds are available for existing algorithms (which are all iterative).

2. Observe that each successive encoder vector has a larger value of the sparsity parameter \( r_j \). In the batch algorithm, every encoder vector has sparsity parameter \( r = 5k + 5k/\varepsilon \) to get a reconstruction error of \((1 + \varepsilon)^2\|X - X_k\|_F^2\). This means that the number of non-zeros in \( H \) is at most \( 5k^2 + 5k^2/\varepsilon \). For the iterative encoder, the first few encoder vectors are very sparse, getting denser as you add more encoder vectors until you get to the last encoder vector which has maximum sparsity parameter \( r_k = 5 + 5k/\varepsilon \). The tradeoff is in the reconstruction error. We can get still sparser in the iterative algorithm, setting every encoder vector’s sparsity to \( r_j = 5 + 5k/\varepsilon \). In this case, the bound on the reconstruction error for \( H_\ell \) becomes \((1 + \varepsilon)^\ell \|X - X_\ell\|_F^2 + \frac{1}{\varepsilon}(1 + \varepsilon)^\ell - 1 \|X_\ell - X_1\|_F^2\), which is growing as \( 1 + O(\varepsilon \ell) \) as opposed to \( 1 + O(\varepsilon \log \ell) \). One other trade off with the iterative algorithm is that the combined sparsity (number of non-zero rows) of \( H \) could increase, as compared to the batch algorithm. In the batch algorithm, the combined sparsity is \( O(k/\varepsilon) \), the same as the sparsity parameter of each encoder vector, since every encoder vector has non-zeros in the same set of rows. With the iterative algorithm, every encoder vector could conceivably have non-zeros in different rows giving \( O(k^2/\varepsilon) \) non-zero rows.

3. Just as with the PCA vectors \( v_1, v_2, \ldots, \), we have an encoder for any choice of \( \ell \) by taking the first \( \ell \) encoder vectors \( h_1, \ldots, h_\ell \). This is not the case for the batch algorithm. If we compute the batch-encoder \( H = [h_1, \ldots, h_k] \), we cannot guarantee that the first encoder vector \( h_1 \) will give a good reconstruction comparable with \( X_1 \).

**Proof.** (Theorem 11) For \( \ell \geq 1 \), we define two quantities \( Q_\ell, P_\ell \) for that will be useful in the proof.

\[
Q_\ell = (1 + \varepsilon)(1 + \frac{1}{2} \varepsilon)(1 + \frac{1}{3} \varepsilon)(1 + \frac{1}{4} \varepsilon) \cdots (1 + \frac{1}{\ell} \varepsilon);
\]

\[
P_\ell = (1 + \varepsilon)(1 + \frac{1}{2} \varepsilon)(1 + \frac{1}{3} \varepsilon)(1 + \frac{1}{4} \varepsilon) \cdots (1 + \frac{1}{\ell} \varepsilon) - 1 = Q_\ell - 1.
\]

Using Lemma 10 and induction, we prove a bound on the information loss of encoder \( H_\ell \):

\[
E \left[ \|X - X H_\ell (X H_\ell)^\dagger X\|_F^2 \right] \leq Q_\ell \|X - X_\ell\|_F^2 + Q_\ell \sum_{j=2}^\ell \frac{P_\ell}{Q_{j-1}}.
\]

(*)
When $\ell = 1$, the claim is that $E[\|X - XH_1(XH_1)\|_F^2] \leq (1 + \varepsilon)\|X - X_1\|_F^2$ (since the summation is empty), which is true by construction of $H_1 = [h_1]$ because $r_1 = 5 + 5/\varepsilon$. Suppose the claim in eq:proof1 holds up to $\ell \geq 1$ and consider $H_{\ell+1} = [h_\ell, h_{\ell+1}]$, where $h_{\ell+1}$ has sparsity $r_{\ell+1} = 5 + 5(\ell + 1)/\varepsilon$. We apply Lemma 10 with $\delta = \varepsilon/(\ell + 1)$ and we condition on $err = \|X - XH_\ell(XH_\ell)^\dagger X\|_F^2$ whose expectation is given in eq:proof1.

By iterated expectation, we have that

$$E \left[\|X - XH_\ell(XH_\ell)^\dagger X\|_F^2\right] \leq (1 + \frac{\varepsilon}{\ell + 1}) E_{H_\ell} \left[\|X - XH_\ell(XH_\ell)^\dagger X\|_F^2 \mid H_\ell\right] \leq \left(1 + \frac{\varepsilon}{\ell + 1}\right) E_{H_\ell} \left[\|X - XH_\ell(XH_\ell)^\dagger X\|_F^2 - \|X - XH_\ell(XH_\ell)^\dagger X\|_F^2\right]$$

$$\leq \frac{Q_{\ell+1}}{Q_\ell} \left(Q_\ell \|X - X_\ell\|_F^2 + Q_\ell \sum_{j=2}^{\ell} \sigma_j^2 \frac{P_{j-1}}{Q_{j-1}} - E_{H_\ell} \left[\|X - XH_\ell(XH_\ell)^\dagger X\|_F^2 \mid H_\ell\right] \geq \sigma_{\ell+1}^2\right)$$

$$= \frac{Q_{\ell+1}}{Q_\ell} \left(Q_\ell \left(\sigma_{\ell+1}^2 + \|X - X_\ell\|_F^2\right) - \sigma_{\ell+1}^2 + Q_\ell \sum_{j=2}^{\ell} \sigma_j^2 \frac{P_{j-1}}{Q_{j-1}}\right)$$

$$= \frac{Q_{\ell+1}}{Q_\ell} \left(Q_\ell \|X - X_\ell\|_F^2 + \sigma_{\ell+1}^2(Q_\ell - 1) + Q_\ell \sum_{j=2}^{\ell} \sigma_j^2 \frac{P_{j-1}}{Q_{j-1}}\right)$$

$$= Q_{\ell+1}\|X - X_\ell\|_F^2 + \sigma_{\ell+1}^2 + Q_{\ell+1} \sum_{j=2}^{\ell+1} \sigma_j^2 \frac{P_{j-1}}{Q_{j-1}}.$$
to obtain the second term in Equation:mainIterative. Observe that for \( i \geq 1 \),
\[
P_i = Q_i - 1 = \varepsilon \frac{Q_i}{Q_1} + \frac{Q_i}{Q_1} - 1 = \varepsilon \frac{Q_i}{Q_1} + P_{i-1},
\]
where we used \( Q_i/Q_1 \leq Q_{i-1} \) and we define \( P_0 = 0 \). Therefore,
\[
\sum_{j=2}^{\ell} \sigma_j^2 \frac{P_{j-1}}{Q_{j-1}} \leq \frac{\varepsilon}{Q_1} \sum_{j=2}^{\ell} \sigma_j^2 + \sum_{j=3}^{\ell} \sigma_j^2 \frac{P_{j-2}}{Q_{j-1}} \leq \frac{\varepsilon}{Q_1} \sum_{j=2}^{\ell} \sigma_j^2 + \sum_{j=3}^{\ell} \sigma_j^2 \frac{P_{j-2}}{Q_{j-2}}.
\]
In (a) we used \( Q_{j-2}/Q_{j-1} < 1 \). The previous derivation gives a reduction from which it is now an elementary task to prove by induction that
\[
\sum_{j=2}^{\ell} \sigma_j^2 \frac{P_{j-1}}{Q_{j-1}} \leq \frac{\varepsilon}{Q_1} \sum_{j=1}^{\ell-1} \|X - X_j\|_F^2.
\]
Since \( \|X - X_j\|_F^2 \leq \|X - X_1\|_F^2 \frac{(\ell - j)}{(\ell - 1)} \), we have that
\[
\sum_{j=2}^{\ell} \sigma_j^2 \frac{P_{j-1}}{Q_{j-1}} \leq \frac{\varepsilon}{Q_1} \sum_{j=1}^{\ell-1} \|X - X_j\|_F^2 \frac{(\ell - j)}{(\ell - 1)} = \frac{\varepsilon}{Q_1} \sum_{j=1}^{\ell-1} \|X - X_j\|_F^2 = \frac{\ell}{2Q_1} \frac{\|X - X_1\|_F^2}{Q_1}.
\]
Using Equation:proof1, we have that
\[
\|X - XH_\ell(XH_\ell)^\dagger X\|_F^2 \leq (\ell \varepsilon) \|X - X_\ell\|_F^2 + \frac{\ell \varepsilon}{2} \|X - X_1\|_F^2 \frac{Q_\ell}{Q_1}.
\]
The result finally follows because
\[
\log \frac{Q_\ell}{Q_1} = \sum_{i=2}^{\ell} \log \left(1 + \frac{\varepsilon}{\ell}\right) \leq \varepsilon \sum_{i=2}^{\ell} \frac{1}{i} \leq \varepsilon (\log(\ell) - 1) = \varepsilon \log \ell,
\]
and so \( Q_\ell/Q_1 \leq \ell^\varepsilon \).

3 Experiments

We compare the empirical performance of our algorithms with some of the existing state-of-the-art sparse PCA methods. The inputs are \( X \in \mathbb{R}^{n \times d} \), the number of components \( k \) and the sparsity parameter \( r \). The output is the sparse encoder \( H = [h_1, h_2, \ldots, h_k] \in \mathbb{R}^{n \times k} \) with \( \|h_i\|_0 \leq r \); \( H \) is used to project \( X \) onto some
subspace to obtain a reconstruction $\hat{X}$ which decomposes the variance into two terms:

$$\|X\|_F^2 = \|X - \hat{X}\|_F^2 + \|\hat{X}\|_F^2$$

\[= \text{Reconstruction Error + Explained Variance}\]

Previous methods construct the matrix $H$ to have orthonormal columns and restrict the reconstruction to symmetric auto-encoders, $\hat{X} = \|XHH^\dagger\|_F^2$. Minimizing the reconstruction error is equivalent to maximizing the explained variance, so one metric that we consider is the (normalized) explained variance of the symmetric auto-encoder,

$$\text{Symmetric Explained Variance} = \frac{\|XHH^\dagger\|_F^2}{\|X_k\|_F^2} \leq 1$$

To capture how informative the sparse components are, we use the normalized information loss:

$$\text{Information Loss} = \frac{\|X - XH(XH)^\dagger X\|_F^2}{\|X - X_k\|_F^2} \geq 1.$$  

The true explained variance when using the optimal decoder will be larger than the symmetric explained variance because $\|X - XHH^\dagger\|_F^2 \geq \|X - XH(XH)^\dagger X\|_F^2$. We report the symmetric explained variance primarily for historical reasons because existing sparse PCA methods have constructed auto-encoders to optimize the symmetric explained variance rather than the true explained variance.

### 3.1 Algorithms

We implemented the following variant of the sparse PCA algorithm of Theorem 7 in the general framework of the algorithm described in Section 2.2: we use the deterministic technique described in part (i) in Theorem 6 in order to find the matrix $C$ with $r$ columns of $X$. (This algorithm gives a constant factor approximation, as opposed to the relative error approximation of the algorithm in Theorem 6 but it is deterministic and simpler to implement.) We call this the “Batch” sparse linear auto-encoder algorithm. We correspondingly implement an “Iterative” version with fixed sparsity $r$ in each principal component. In each step of the iterative sparse auto-encoder algorithm we use the above batch algorithm to select one principal component with sparsity at most $r$.

We compare our sparse auto-encoder algorithms to the following state-of-the-art sparse PCA algorithms:

1. **TPower**: This is the truncated power method for sparse PCA described in [Yuan and Zhang, 2013].
2. **Gpower-$\ell_0$**: This is the generalized power method with $\ell_0$ minimization in [Journé et al., 2010].
3. **Gpower-$\ell_1$**: This is the generalized power method with $\ell_1$ minimization in [Journé et al., 2010].

All those algorithms were designed to operate for the simple $k = 1$ case (notice that our algorithms handle any $k$ without any modification); hence, to pick $k$ sparse components, we use the “deflation” method suggested in [Mackey, 2009]: let’s say $h_1$ is the result of some method applied to $X$, then $h_2$ is the result of the same method applied to $(I_n - h_1h_1^\dagger) \cdot X \cdot (I_n - h_1h_1^\dagger)$, etc.
3.2 Environment, implementations, datasets

We implemented our sparse linear auto-encoder algorithms in Matlab. For all the other algorithms, we used the matlab implementations from Yuan and Zhang [2013]. The implementations of the GPower method with $\ell_1$ or $\ell_0$ minimization is from the original paper Journee et al. [2010]. We run all the experiments in Matlab 8.4.0.150421 (R2014b) in a Macbook machine with 2.6 GHz Intel Core i7 processor and 16 GB of RAM.

Following existing literature, we test the above algorithms in the following three datasets (all available in Yuan and Zhang [2013]): 1) PitProps: Here, $X \in \mathbb{R}^{180 \times 13}$ with $n = 13$ corresponds to a correlation matrix of 180 observations measured with 13 variables. The original dataset is described in Jeffers [1967]. 2) Colon: This is the gene-expression dataset from Alon et al. [1999]; here, $X \in \mathbb{R}^{500 \times 500}$. 3) Lymphoma: This is the gene-expression dataset from Alizadeh et al. [2000]; here, $X \in \mathbb{R}^{500 \times 500}$. Those are PSD matrices, hence fit the sparse PCA framework we discussed above.

3.3 Results

For each dataset, we tried different $k$ and the sparsity $r$. The qualitative results for different $k$ are similar so we only show results for $k = 2$. We report the results in Figure 1. Notice that we plot the symmetric explained variance and the information loss versus the “average column sparsity” of $H$. This is because all algorithms - with TPower being an exception - cannot guarantee column sparsity in $H$ of exactly $r$, for
given $r$. Our methods, for example, promise column sparsity at most $r$. The GPower methods control the sparsity level through a real parameter $\gamma$ which takes values in $(0,1)$. An exact relation between $\gamma$ and $r$ is not specified, hence we experimented with different values of $\gamma$ in order to achieve different levels of sparsity.

We show example sparse encoders $H = [h_1, h_2]$ for the 5 algorithms with $k = 2$ and $r = 5$ below

| Batch | Iter. | TP | GP-$\ell_0$ | GP-$\ell_1$ |
|-------|-------|----|-------------|-------------|
| $h_1$ | $h_2$ | $h_1$ | $h_2$ | $h_1$ | $h_2$ | $h_1$ | $h_2$ |
| 0 0 | -0.8 -0.3 | 0 0 | 0.5 0 | 0.7 0 | 0.6 0 |
| 0 0 | 0 -0.4 | 0 0 | 0.6 0 | 0.7 0 | 0.7 0 |
| 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 |
| 0 0 | 0 0 | 0 0 | 0.3 0 | 0 0 | 0 0 |
| 0 0 | 0 0 | 0 0 | 0 0 | 0 0 | 0 0 |

The sparse encoder vectors differ significantly among the methods. This hints at how sensitive the optimal solution is, which underlines why it is important to optimize the correct loss criterion. Since one goal of low-dimensional feature construction is to preserve as much information as possible, the information loss is the compelling metric.

Our algorithms give better information loss than existing sparse PCA approaches. However, existing approaches have higher symmetric explained variance. This is in general true across all three datasets and different values of $k$. These findings shouldn’t come at a surprise, since previous methods aim at optimizing symmetric explained variance and our methods choose an encoder which optimizes information loss. The figures highlight once again how different the solutions can be. It also appears that our “iterative” algorithm gives better empirical information loss compared to the batch algorithm, for comparable levels of average sparsity, despite having a worse theoretical guarantee.

Finally, we mention that we have not attempted to optimize the running times (theoretically or empirically) of our algorithms. Faster versions of our proposed algorithms might give as accurate results as the versions we have implemented but with considerably faster running times; for example, in the iterative algorithm (which calls the CSSP algorithm with $k = 1$), it should be possible significantly speed up the generic algorithm (for arbitrary $k$) to a specialized one for $k = 1$. We leave such implementation optimizations for future work.
4 Discussion

Historically, sparse PCA has meant cardinality constrained variance maximization. Variance per se does not have any intrinsic value, and it is not easy to generalize to arbitrary encoders which are either not orthogonal or not decorrelated. However, the information loss is a natural criterion to optimize because it directly reflects how good the features are at preserving the data. Information loss captures the machine learning goal when reducing the dimension: preserve as much information as possible.

We have given efficient asymptotically optimal sparse linear encoders An interesting open question is whether one can get a \((1 + \epsilon)\)-relative error with respect to information loss for the iterative encoder. We believe the answer is yes as is evidenced by the empirical performance of the iterative encoder.

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