ReFACTor: Practical Low-Rank Matrix Estimation Under Column-Sparsity

Matan Gavish*,1, Regev Schweiger*,2, Elior Rahmani2 and Eran Halperin3,4

*Equal contribution
1School of Computer Science and Engineering, Hebrew University of Jerusalem, Jerusalem, Israel
2Blavatnik School of Computer Science, Tel Aviv University, Tel Aviv, Israel
3Department of Computer Science, University of California, Los Angeles, CA, USA
4Department of Anesthesiology and Perioperative Medicine, University of California, Los Angeles, CA, USA

Abstract

Various problems in data analysis and statistical genetics call for recovery of a column-sparse, low-rank matrix from noisy observations. We propose ReFACTor, a simple variation of the classical Truncated Singular Value Decomposition (TSVD) algorithm. In contrast to previous sparse principal component analysis (PCA) algorithms, our algorithm can provably reveal a low-rank signal matrix better, and often significantly better, than the widely used TSVD, making it the algorithm of choice whenever column-sparsity is suspected. Empirically, we observe that ReFACTor consistently outperforms TSVD even when the underlying signal is not sparse, suggesting that it is generally safe to use ReFACTor instead of TSVD and PCA. The algorithm is extremely simple to implement and its running time is dominated by the runtime of PCA, making it as practical as standard principal component analysis.

1 Introduction

Principal Component Analysis (PCA) or Truncated Singular Value Decomposition (TSVD) are arguably among the most ubiquitous methods used for data analysis in science and engineering [1–5]. The main objective of these methods is to search for low rank signals hidden in a data matrix. Formally, suppose that \( X \) is an unknown low rank \( m \)-by-\( n \) matrix. We observe a single noisy \( m \)-by-\( n \) matrix \( Y \), obeying \( Y = X + \sigma Z \), where \( Z \) is an unknown noise matrix and \( \sigma > 0 \) is the noise level. Our goal is to estimate \( X \) from the data \( Y \). Using the Singular Value Decomposition (SVD) of \( Y \), we can write

\[
Y = \sum_{i=1}^{m} y_i u_i v_i^\top
\]

where \( u_i \in \mathbb{R}^m \) and \( v_i \in \mathbb{R}^n \), \( i = 1, \ldots, m \) are the left and right singular vectors corresponding to the singular value \( y_i \). The TSVD estimator [6] is

\[
\hat{X}_r = \sum_{i=1}^{r} y_i u_i v_i^\top,
\]

where \( r = \text{rank}(X) \) assumed known, and \( y_1 \geq \ldots \geq y_m \). One of the appealing properties of TSVD, which helped it gain popularity, is that the estimator \( \hat{X}_r \) is the best possible approximation of rank \( r \) to the data matrix \( Y \) in the least squares sense [7], and therefore the maximum likelihood estimator under Gaussian noise. We note, however, that \( \hat{X}_r \) is not necessarily the best approximation for the signal matrix \( X \), which is in essence more relevant [8].
Column sparsity. The implicit likelihood model solved by TSVD assumes that the entries of $Z$ are independent and normally distributed, but it does not make any assumptions on the matrix $X$. In many applications, there is additional information about the underlying signal matrix $X$ that can be leveraged for estimation. Particularly, it is sometimes the case that $X$ is a column-sparse matrix, meaning that all but $t$ columns of $X$ are zero. We call the non-zero columns of $X$ active columns, and the other columns non-active. Equivalently, the right singular vectors of $X$ are all sparse, with a common same sparsity pattern. This kind of data emerges in various domains. In recommendation systems, estimation of a user-item preference matrix when certain blocks of users are indifferent to some of the items, or when some columns are outlier measurements [9]; In signal processing and array processing, denoising of a signal measured over time, which is either intermittent or contaminated by an intermittent interference [10]; In genomics, and specifically in DNA methylation, estimation of strong systematic confounders poses a key challenge that is well modeled by estimation of a column-sparse matrix. In Section 6 below, we focus on DNA methylation and provide a detailed, real data example of this application.

Connections with Sparse PCA. Estimation of column-sparse matrices is closely related to sparse PCA. There, one is interested in estimating the eigenvectors of $X^TX$ or $XX^T$ (assumed sparse), or their support (not assumed to be common for all vectors), rather than estimating the matrix $X$ itself; this makes sparse PCA a different, and in some sense, a harder problem than the one we address. Sparse PCA has received considerable attention in the machine learning and statistics communities, owing to a fascinating combination of statistical hardness and computational hardness [11–20]. The fundamental limits for consistent support estimation are known [20–22], as are the minimax rates [17, 23–25]. It is natural to ask whether sparse PCA algorithms can be “lifted” into estimators of column-sparse matrices. Unfortunately, many of the algorithms proposed are not computationally feasible for real-life datasets, or may be difficult to implement or use (e.g., using semidefinite programming [15, 19, 26] or other optimization techniques [17, 25, 27]). Other methods are heuristic in nature in the sense that there are no provable guarantees that they will provide improved estimates of the eigenvectors (and therefore of $X$), and indeed it is not known whether they outperform even the simplest approach where one applies TSVD. There are a few exceptions, where simple and computationally efficient methods are analyzed and shown to perform better than PCA. Particularly, [14] proposes a method to detect the active columns of $X$, and they show that in the limit, their algorithm provides a consistent estimate of the top singular vector under the assumption that $m/n \to \beta$, where $\beta > 0$ is a constant. Moreover, [15] analyze the algorithm of [14] and show that it successfully recovers the $t$ active columns of $X$ if $t \leq O(\sqrt{m/\log n})$ when $r = 1$ and the singular vector of $X$ has entry $1/\sqrt{t}$ in each of the active columns. [19] studied covariance thresholding, again for estimating the top eigenvalues of $XX^T$, yet is not immediately clear how their methods can be used for direct estimation of a column-sparse $X$.

Motivation: A simple, practical algorithm with theoretical guarantees. Our motivation for the algorithm suggested here is based on the gap between practice and theory. In practice, most researchers in science that use PCA or SVD do not use the sparse versions since the algorithms are either too complex or are not necessarily guaranteeing an improved performance. The algorithm of [14] is an example for a simple procedure that would be easy to apply by any practitioner, as it merely computes the norm of each column of the data matrix $Y$ and then computes SVD on the columns with the largest norms. Their method, as well as its inherent over-sensitivity to arbitrary scaling of the columns, is described in more details in Section 3 below. Other methods such as [18] assume non-negative entries in the matrix $X$, a problematic assumption in most practical instances, and particularly in the two example applications above.

The algorithm. In this paper we introduce ReFACTor – a simple modification of TSVD, which is designed to outperform the original on column-sparse data while still being safe to use even without column-sparsity. Our algorithm is extremely simple, so that it is more likely to be used correctly by practitioners, who are familiar with PCA and SVD, but who may be hesitant to adapt more complicated methods.

For any matrix $X$, let $[X]_r$ denote the $j$-th column of $X$. Assuming oracle knowledge of the underlying $r$ and the column-sparsity $t$, the ReFACTor estimator proceeds in three steps:

1. Compute the TSVD $\hat{X}_r$ of the data $Y$. 

2. Compute the $t$ largest singular values of $\hat{X}_r$. 

3. Compute the $t$ largest left singular vectors of $\hat{X}_r$. 


2. Compute the column scalar products \( c_j = \langle [\hat{X}_r]_{j}, [Y]_j \rangle \) and sort them in absolute value to obtain \( |c_{j(1)}| \geq |c_{j(2)}| \geq \ldots \geq |c_{j(n)}| \). Here, \((j(1), \ldots, j(n))\) is a permutation of \((1, \ldots, n)\).

3. Keep the first \( t \) columns with largest absolute scalar products, namely \([\hat{X}_r]_{j(i)}\) with \(1 \leq i \leq t\), and set to zero the rest. Formally,

\[
[\hat{X}_{r,t}^RF]_{j(i)} = \begin{cases} 
[\hat{X}_r]_{j(i)} & 1 \leq i \leq t \\
0 & t + 1 \leq i \leq n 
\end{cases},
\]

where \(\hat{X}_{r,t}^RF\) is the ReFACTor estimator, with tuning parameters \(r, t \in \mathbb{N}\).

When \(r\) is understood, we write simply \(\hat{X}_t^RF\).

A preliminary empirical observation. Our basic algorithm admits several natural variations. First, we can replace the inner products \( c_j \) in step 2 with correlations between columns

\[
c_j^+ = \frac{\langle [\hat{X}_r]_{j}, [Y]_j \rangle}{\| [\hat{X}_r]_j \| \cdot \| [Y]_j \|},
\]

sort them, and let the rest of the algorithm proceed as before. Importantly, this makes the algorithm insensitive to individual column scaling. We call this variation of the algorithm ReFACTor+. Second, instead of returning \(\hat{X}_{r,t}^RF\) we can return the TSVD of the matrix \(\tilde{Y}\) with

\[
[Y]_{j(i)} = \begin{cases} 
[Y]_{j(i)} & 1 \leq i \leq t \\
0 & t + 1 \leq i \leq n 
\end{cases}.
\]

Let us call this variation the algorithm ReFACTor*.

Recently, it was shown that ReFACTor* is extremely efficient in removing strong systematic confounders from DNA methylation data [28]. The algorithm was presented there as a heuristic; in this paper we undertake to analyze its merits formally and explain its success. It is harder to analyze ReFACTor*, but as we show in Section 5 below, its performance is empirically similar to that of ReFACTor and ReFACTor+. Thus, in this short paper we primarily study the simpler ReFACTor and ReFACTor+ algorithms.

Synopsis. Let us measure the performance of an estimator \(\hat{X} = \hat{X}(Y)\) for \(X\) by expected mean square error (MSE). In our case, this is just the Frobenius loss

\[
\| \hat{X}(Y) - X \|_F^2,
\]

where \(\| \cdot \|_F^2\) is the sum of squares of matrix entries. The TSVD estimator \(\hat{X}_r\) is an optimal rank-\(r\) approximation of the data matrix \(Y\), in MSE, yet there is no a-priori reason why it should be a good, or even reasonable, estimator for the signal matrix \(X\). Indeed when \(r \ll n\) it was shown to be significantly suboptimal [8].

In this paper we prove that, when \(X\) is low rank and column-sparse, the ReFACTor estimator \(\hat{X}_{r,t}^RF\) is as good as the traditional TSVD \(\hat{X}\), or better. Formally, with high probability,

\[
\| \hat{X}_{r,t}^RF - X \|_F^2 \leq \| \hat{X}_r - X \|_F^2.
\]

In other words, when column-sparsity is known to hold, the simple procedure of removing columns of the TSVD with low correlations with the data matrix is safe to use, as it can only improve estimation. We further prove that the relative improvement in MSE can be quite substantial. In the Supporting Information, we prove analogous results for ReFACTor+. (We note that ReFACTor+ is much more useful in practice, since ReFACTor is sensitive to an arbitrary scaling of the columns.) Interestingly, we bring solid empirical evidence that ReFACTor always offers improved MSE relative to the TSVD baseline, regardless of the underlying column sparsity.
2 Setup and notation

Column vectors are denoted by boldface letters such as \( \mathbf{v} \), their transpose by \( \mathbf{v}^\top \) and their coordinates e.g. by \( v = (v_1, \ldots, v_m)^\top \). Let

\[
X = \sum_{i=1}^{r} x_i \mathbf{a}_i \mathbf{b}_i^\top
\]

be a Singular Value Decomposition of the signal matrix \( X \) we wish to estimate. Here, \( \mathbf{a}_i = ((a_{i1}), \ldots, (a_{im}))^\top \in \mathbb{R}^m \) and \( \mathbf{b}_i = ((b_{i1}), \ldots, (b_{in})) \in \mathbb{R}^n \) are all unit vectors. For column sparsity, we may reorder the columns if necessary and assume that \( [X]_{ij} = 0 \) for \( j > t \). This implies \( (b_{ij}) = 0 \) for \( j > t \) and all \( i \). The data matrix available to us is \( Y = X + (\sigma/\sqrt{n})Z \) where \( Z \) is an \( m \)-by-\( n \) matrix whose entries are \( Z_{ij} \sim \mathcal{N}(0,1) \). (This noise normalization is standard in matrix denoising, as it prevents the singular values of \( Z \) from growing with \( n \), keeping a fixed signal-to-noise ratio.) Throughout this paper, the index \( i \) will be used for singular values and vectors, and the index \( j \) will be used for columns. For example, \( (v_i)_j \) is the \( j \)-th coordinate of the \( i \)-th singular vector \( v_i \).

Finally, throughout the paper, we will say that an event \( A_n \) occurs with high probability if \( \Pr(A_n) = 1 - O(1/n) \). The parameter \( n \) in the context of this paper corresponds to the number of columns of the matrix. Note that if \( A_n, B_n \) occur with high probability then \( A_n \land B_n \) also occurs with high probability.

3 Merits of the ReFACTor statistic

Under the “prior” that only \( t \) columns of \( X \) are nonzero, denoising of \( X \) is much better done on the active columns alone, namely those columns \( j \) where \( [X]_{ij} \neq 0 \). Therefore, a reasonable denoising algorithm will proceed in two steps: First, detect active columns; Second, denoise using active columns only, and estimate those columns that were detected to be non-active by 0. A natural method for detecting the active columns is due to [14]. They considered the simple statistic

\[
T_{\chi}^X = ||[Y]_{j}||^2.
\]

For non-active columns, this statistic is distributed \( \chi^2_m \), while for active columns it is distributed \( \chi^2_m \left( ||[X]_{j}||^2 \right) \), the latter denoting the non-central \( \chi^2 \) on \( m \) degrees of freedom with noncentrality parameter \( ||[X]_{j}||^2 \). Detection of the active columns would then proceed by testing the hypothesis that the noncentrality parameter is zero for each column.

This method does not capitalize on the low-rank assumption. To see why, observe that

\[
T_{\chi}^X = \langle [Y]_{j} \rangle^2 \langle [Y]_{j} \rangle
\]

\[
= \left( \sum_{i=1}^{m} y_i \mathbf{u}_i (v_{ij}) \right)^2 \left( \sum_{k=1}^{m} y_k \mathbf{u}_k (v_{kj}) \right)
\]

\[
= \sum_{i,k=1}^{m} y_i y_k (v_{ij}) (v_{kj}) \langle \mathbf{u}_i, \mathbf{u}_k \rangle
\]

\[
= \sum_{i=1}^{m} y_i^2 (v_{ij})^2.
\]

It follows that

\[
T_{\chi}^X = \sum_{i=1}^{r} y_i^2 (v_{ij})^2 + \sum_{i=r+1}^{m} y_i^2 (v_{ij})^2.
\]
When \( \text{rank}(X) = r \ll m \), the first \( r \) right singular vectors hold information regarding \( X \), while all the rest are just noise. The same is true for the singular values. Therefore the left sum in (6) contains the signal and the right sum contains noise which harms the detection.

In contrast, the ReFACTor algorithm detects active columns based on the statistic
\[
T_j^{RF} = \langle [Y]_j, [\hat{X}]_j \rangle.
\]

The calculation above readily shows that
\[
T_j^{RF} = \sum_{i=1}^{r} y_i^2 (v_i)_j^2,
\]
capturing only the “signal” part of \( T_j^X \).

4 Main results

Following [14, 15], we study formally the case \( r = 1 \). As these authors note, this case offers all the insight of the general case, while allowing proofs to be reasonably readable and understandable. Let \( a \equiv a_1 \) and \( b \equiv b_1 \), with entries \((a_1, \ldots, a_m)\) and \((b_1, \ldots, b_n)\) respectively. Similarly let \( u \equiv u_1 \) and \( v \equiv v_1 \) with entries \((u_1, \ldots, u_m)\) and \((v_1, \ldots, v_n)\). Also write \( y \equiv y_1 \) for the leading data singular value and \( x \equiv x_1 \) for the leading original singular value. We simplify and write \( \hat{X}_{RF} \) for \( \hat{X}_{RF}^{r,t} \) with \( r = 1 \). As before, \( \hat{X}_1 \) denotes the truncated SVD with \( r = 1 \).

Theorem 1. ReFACTor is better when the signal is not too weak. Assume that \( x > \sqrt{1 + 2\sqrt{\beta}} \), where \( \beta = m/n \). There exists a constant \( C \) such that if for all \( j = 1, \ldots, t \) we have
\[
b_j^2 > C \frac{\log n}{n},
\]
then, with high probability
\[
\| \hat{X}_t^{RF} - X \|_F^2 \leq \| \hat{X}_1 - X \|_F^2.
\]

Interestingly, this theorem does not explicitly assume anything about the sparsity \( t \). When \( t \) is not large, the condition \( b_j^2 > C \log n/n \) is quite mild, since there are only \( t \) nonzero entries.

In fact, the relative gain in MSE offered by \( \hat{X}_t^{RF} \) with respect to \( \hat{X}_1 \) is quite massive:

Theorem 2. Relative improvement in MSE. Make the same assumptions as in Theorem 1. For every fixed \( \epsilon > 0 \), with high probability we have for the relative improvement in MSE
\[
\frac{\| \hat{X}_1 - X \|_F^2 - \| \hat{X}_t^{RF} - X \|_F^2}{\| X \|_F^2} \geq 1 - \frac{t + \log n}{n} (1 + \epsilon).
\]

Even without any assumption on the signal singular vector, a mild sparsity assumption is enough to guarantee that ReFACTor can only improve estimation:

Theorem 3. Even under mild column sparsity, ReFACTor is better. Assume that \( x > \sqrt{1 + 2\sqrt{\beta}} \). There exists a constant \( C_0 \) such that if
\[
t \leq C_0 \frac{n}{\log n}
\]
then with high probability
\[
\| \hat{X}_t^{RF} - X \|_F^2 \leq \| \hat{X}_1 - X \|_F^2.
\]

Analogous results for ReFACTor+. In the Supporting Information we prove analogous results for ReFACTor+, which we omit here due to space limitations.
5 Simulation study

We performed a comprehensive simulation study, comparing \textit{ReFACTor}, \textit{ReFACTor}$^*$ and \textit{ReFACTor}+ to the baseline TSVD $\hat{X}$ of (2). We also compared two algorithms based on the method of [14] for detecting “active” columns. Specifically, let $j(1), \ldots, j(t)$ be the indices of the $t$ columns of $Y$ with the largest value of $||[Y]_j||^2$. Let $JL$ be the algorithm that uses (3) to estimate $X$, and let $JL^*$ be the algorithm that returns the TSVD of the matrix as in (4). We chose a fixed noise level $\sigma = 1$. In each simulation, we scanned over a range of values for $x$ (the signal singular value), $n$ (the number of columns, with number of rows $m$ being held fixed) and column sparsity $t$ (with the number of columns $n$ being held fixed). These scans were performed for different values of the underlying $r = \text{rank}(X)$ and with the entries of the noise matrix $Z$ sampled from different noise distributions. The full results of our simulation study span some 98 figures, and are shown in the Supporting Information. Sample results are shown in Figure 1, Figure 2 and Figure 3.

![Figure 1](image)

**Figure 1:** The performance of \textit{ReFACTor}, TSVD and \textit{JL} on a $200 \times 200$ matrix of Gaussian noise, with $x = 4$, $r = 5$. The number of active columns, $t$, is varied, and performance is measured by the MSE of the estimated matrix, averaged across 50 runs. \textit{ReFACTor} consistently outperforms the other algorithms across the entire measured range.

Inspection of the empirical evidence suggests the following:

\textbf{ReFACTor is safe to use.} When the true column sparsity is known, and when the singular value $x$ is strong enough (in the sense of Theorems 1 and 3), \textit{ReFACTor} offers MSE that is \textit{always} less than or equal, and often noticeably smaller than the MSE of the baseline TSVD (Figures 1, 2 and 3). For a high $r$ (e.g., $r = 40$ for $m = n = 200, t = 100$), the performance of \textit{ReFACTor} and \textit{JL} is nearly identical. This shows that even when the low rank assumption on which \textit{ReFACTor} capitalizes does not hold, it does not suffer from a performance loss.

\textbf{ReFACTor is preferred to JL if $x$ is not weak.} For all values of $x$, except values close to the BBP phase transition\footnote{The BBP phase transition [29, 30] is a phenomenon describing the behaviour of the largest singular value of perturbations of low rank by large rectangular random matrices. It describes a threshold for the largest singular value, depending on matrix size and on the noise distribution, under which the unperturbed singular values and vectors cannot be estimated. In the context of Gaussian noise, this threshold is $\beta^{-1/4}$.}, \textit{ReFACTor} is preferred to \textit{JL} (Figure 2). This is in line with the Discussion above; indeed, when the signal of $x$ is weak, it is spread across the entire space, giving \textit{JL} a slight advantage.

\textbf{Algorithm variations do not matter much.} The performance of the \textit{ReFACTor}$^*$ (resp. \textit{JL}$^*$) variant is very close to that of \textit{ReFACTor} (resp. \textit{JL}), as seen in Figure 3. Similarly, the performance of \textit{ReFACTor}$^+$ is...
almost identical to that of ReFACT or. This is particularly advantageous in practice, since both ReFACT or and JL are sensitive to arbitrary scaling of the columns.

The theoretical requirements are not tight. The algorithm works well even outside the scope of our theoretical results.

Universality: Results do not depend on the noise distribution. Performance results do not qualitatively change as the distribution of the i.i.d. noise is changed, implying a more universal validity to our results.

6 Real data example: DNA methylation

DNA methylation is the phenomenon whereby a methyl group is attached to specific sites in the DNA [31]. A typical DNA methylation study generates an $m$-by-$n$ data matrix $Y$, with measurements of DNA methylation on $m$ subjects at $n$ genomic sites, such that $Y_{i,j} \in [0, 1]$ the fraction of cells of individual $i$ that are methylated in position $j$ in the genome. In a typical study, the scientist is interested in the correlation of one or more $m$-by-1 disease status vectors $y$ with each of the columns of $Y$. Before interesting correlations with disease vectors can be detected, the scientist must remove strong systematic confounders from the data. Modeling the measurements as $Y = X + \sigma Z$, where $X$ is a low-rank matrix of strong systematic confounders, the scientist must first form an estimate $\hat{X}$ of $X$, and use the column space of $\hat{X}$ to test for significant correlations between $y$ and the columns of $Y$, after deducting the contribution of the confounders.

It was recently shown [32] that a leading source of strong systematic confounders is cell type composition. Most studies to date have been performed on whole-blood samples; however, blood is a heterogeneous collection of different cell types, each with a different typical methylation profile. Indeed, the top left singular vectors of $Y$ have been shown to be strongly correlated with the cell type composition in blood [33]. If a disease status $y$ is correlated with the cell type composition (as is the case in many diseases), then $y$ will be correlated with columns in which the typical methylation is different across different cell types. These associations do not indicate a specific connection between a methylation site and the trait.

If cell type counts were available for each individual, one could regress out the influence of cell type
Figure 3: The performance of ReFACTor, TSVD and JL on a 200 × 200 matrix of Gaussian noise, with $x = 4$ and in a low rank setting, with $r = 1$. The number of active columns, $t$, is varied, and performance (MSE) is measured by the Frobenius norm of the difference between the estimated matrix to the original. Standard errors not shown for clarity of presentation. The improvement of ReFACTor over TSVD and JL is more substantial in a low rank setting. Additionally, the ReFACTor*, ReFACTor+ and JL* variations do not display a significant difference in performance here relative to their respective counterparts.

composition from each methylation site measurement in order to account for this confounder. In their absence, one could instead regress out the top principal components, which behave as a surrogate for the cell counts. Recently, it has been shown [28] that sparse PCA results in a much better prediction of the blood cell counts compared to standard PCA. This is mainly because only a subset of methylation sites are differentially methylated across cell types. The algorithm used in [28] is highly similar to the algorithm presented here. However, its use has been heuristic without any theoretical guarantees. This work aims to provide theoretical guarantees to a slight modification of that algorithm.

To demonstrate the presence of sparse principal components in methylation data, we used the data of [34], in which a methylation matrix $Y$ of 686 individuals by 103,638 sites is provided. In addition, a boolean phenotype vector $y$ of length 686 is provided, indicating for each individual if they were diagnosed with Rheumatoid Arthritis (RA). Here, we assume $r = 1$; that is, that a single cell type dominates the confounding signal [28]. Let $X$ be the rank-1 matrix whose elements $X_{i,j}$ indicate, for the $i$-th individual and for the $j$-th site, the proportion of the single cell type for the individual, multiplied by the typical difference of methylation level between the dominating cell type and other cell types, for that site [28].

Under the assumption that $Y = X + \sigma Z$, where $X$ is a low rank signal matrix with significant column sparsity, if $y$ is correlated with the left singular vector of $X$ then $y$ will be correlated with the active columns of $X$. We thus estimate the left singular vector of $X$ using either ReFACTor*, TSVD or JL*. (Results using ReFACTor+ are similar and are not shown here.) Given such an estimate, we remove from each column of $Y$ its projection on this vector. If the estimate is accurate, the transformed columns of $Y$ will be uncorrelated with $y$. We estimate the correlation between each transformed column of $Y$ and $y$ using logistic regression, which results in a p-value per column, calculated by a standard Wald test. Assuming an accurate estimate, we expect the distribution of the p-values to be approximately uniform, perhaps with very few outliers which might indicate true correlations. As shown in Figure 4, indeed, ReFACTor (with $r = 1$) empirically results in a relatively uniform p-value distribution, while the other methods tend to result in many significant p-values. A full description of the experiment is available at the Supplementary Information.
Figure 4: Results of the real data Rheumatoid Arthritis methylation analysis, presented by quantile-quantile plots of the $-\log_{10}(p)$-values for the association tests. Significant deviation from the black line indicates an inflation arising from a confounder in the data. Results are shown for ReFACTor*, TSVD and JL*. Estimating the effect of cell type composition using ReFACTor* results in a significantly lower inflation.

7 Proof setup and useful Lemmas

For $r = 1$, the detection statistic used by ReFACTor is simply

$$T^{RF}_j = y^2 v^2_j.$$  

The ReFACTor algorithm sorts the values $\{T^{RF}_j\}_{j=1}^n$ and picks the $t$ columns with the largest value of the detection statistic. Equivalently, the algorithm sorts the values $(v_1^2, \ldots, v_n^2)$ and picks the $t$ columns with the largest values. Let $w$ denote the projection of $v$ on $b^\perp$, so that

$$v = c \cdot b + s \cdot w,$$

with

$$c = \langle v, b \rangle \quad s = \|v - \langle v, b \rangle b\|.$$

and $c^2 + s^2 = 1$. We write $(w_1, \ldots, w_n)$ for the coordinates of $w$.

Let us first characterize the distribution of the entries of $w$.

**Lemma 1. Marginal distribution of the entries of $w$.** Let $w_j$ be the $j$-th entry of $w$ from (8), namely the projection of $v$ on $b^\perp$. Let $\tilde{w} \sim N(0, I - bb^\top)$. Then for $j = 1, \ldots n$, $w_j$ jointly have the same distribution as

$$\frac{\tilde{w}_j}{\sqrt{\sum_{j=1}^n \tilde{w}^2_j}}$$

and $\sum_{j=1}^n \tilde{w}_j^2 \sim \chi^2_{n-1}$.

Toward our main result, we show that the entries of $v$ on active and non-active columns differ substantially.

**Lemma 2. Right singular vector is small in inactive columns.** Let $j > t$ and $\alpha > 1$. Then

$$Pr \left( v_j^2 > \frac{s^2 \alpha^2 \log n}{n} \right) \leq \frac{2}{n^{\alpha^2/2}}.$$
Lemma 3. Right singular vector is large in active columns. Let \( j \leq t \) and \( \alpha > 1 \). Assume that

\[
b_j^2 \geq \frac{4s^2 \alpha^2 \log n}{c^2 n}.
\]

Then

\[
\Pr \left\{ v_j^2 < \frac{s^2 \alpha^2 \log n}{n} \right\} \leq \frac{2}{n^{\alpha^2/8}}.
\]

We next show that when the signal singular value \( x \) is strong enough, the cosine \( c \) from (8), namely the cosine of the angle between \( b \) and \( v \), is not too small.

Lemma 4. A lower bound on the cosine. Let \( x > \sqrt{1 + 2\sqrt{\beta}} \). Then with high probability \( c^2 \geq \frac{1}{2} \).

Finally, we show that the singular value in \( Y \) is larger than the original singular value, with high probability.

Lemma 5. A lower bound on the singular value. Let \( x, y \) be defined as above. Then with high probability \( y > x \).

The following are auxiliary lemmas needed for our main results.

Lemma 6. Let \( X \sim \chi^2_m \). Then, we have \( \Pr(X \leq (1 - \epsilon)m) \leq e^{-x^2m} \). Also, for every \( 0 < \epsilon < 2 \), we have \( \Pr(X \geq (1 + \epsilon)m) \leq e^{-x^2m/8} \).

Lemma 7. Let \( w_1, \ldots, w_m \sim \mathcal{N}(0, 1) \) be independent standard normal random variables, and let \( w_{(1)}, \ldots, w_{(m)} \) be their order statistics. Let \( \delta > 0 \) be a fixed constant. There is a constant \( C > 0 \), such that for \( t \leq (1 - \delta)m \), with high probability \( w_{(1)} + \cdots + w_{(m-t)} > Cm \).

8 Proofs

For space considerations, proofs of Theorem 2 and all Lemmas are deferred to the Supporting Information.

Proof of Theorem 1. It is easy to see that for \( \alpha = 4 \), Lemmas 2 and 3 hold with probability at least \( 1 - O(1/n^2) \) for all columns \( j = 1, \ldots, n \). In addition, by Lemma 4, with high probability \( s^2 \leq c^2 \). Thus, letting \( C = 4\alpha^2 \), with high probability for any \( j \leq t \) we have \( b_j^2 \geq C \log n/n \geq 4s^2 \alpha^2 \log n/c^2 n \). By Lemma 2 and Lemma 3, the value of \( v_j^2 \) on any active column is larger than \( v_j^2 \) on any inactive column with high probability, so that ReFACToR correctly identifies the active columns. In other words, \( \hat{X}^{RF}_j = [X]_j = 0 \) on \( j > t \), implying

\[
\left\| \hat{X}^{RF}_t - X \right\|_F^2 = \sum_{j=1}^t \left\| \hat{X}_1_j - [X]_j \right\|_F^2 \leq \sum_{j=1}^n \left\| \hat{X}_1_j - [X]_j \right\|_F^2
\]

as required. \( \Box \)

Proof of Theorem 3. Let \( R^+ = \{j(1), \ldots, j(t)\} \) denote the set of \( t \) indices detected as active by \( T^{RF} \) and let \( R^- = \{1, \ldots, n\} \setminus R^+ \) denote the indices detected as inactive. Define \( R^{++} = \{1, \ldots, t\} \cap R^+ \) (true positive detections), \( R^{+-} = \{1, \ldots, t\} \cap R^- \) (false negative detections), \( R^{-+} = \{t + 1, \ldots, n\} \cap R^+ \) (false positive detections), \( R^{--} = \{t + 1, \ldots, n\} \cap R^- \) (true negative detections). For any set of indices \( R \) let

\[
\Delta(R) = \sum_{j \in R} \left\| \hat{X}^{RF}_j - [X]_j \right\|_F^2 - \sum_{j \in R} \left\| \hat{X}_1_j - [X]_j \right\|_F^2
\]

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denote the gain in MSE over the columns in $R$. Clearly $\Delta(R^{++}) = \Delta(R^{-+}) = 0$. It remains to show that $\Delta(R^{++}) + \Delta(R^{-+}) < 0$ with high probability.

First, we bound from below the gain from true negatives. It can be easy seen that $\Delta(R^{-+}) = -y^2 \sum_{j \in R^{-+}} v_j^2$. Denote by $J$ the set of indices of the $n - 2t$ smallest values from $v_{t+1}^2, \ldots, v_n^2$, or equivalently, from $\tilde{w}_{t+1}^2, \ldots, \tilde{w}_n^2$. Since there are at least $n - 2t$ indices in $R^{-+}$, and since ReFACTors detects as inactive the smallest values of the vector $v$, we have $J \subseteq R^{-+}$. Since $t = O(n/\log n)$, by Lemma 7, there exists $C > 0$ so that with high probability

$$\sum_{j \in R^{-+}} \tilde{w}_j^2 \geq C n$$

Additionally, by Lemma 6, with high probability $\|\tilde{w}\|^2 \leq 2n$. Therefore, since $v_j^2 = s^2 \tilde{w}_j^2/\|\tilde{w}\|^2$, with high probability

$$\sum_{j \in R^{-+}} v_j^2 \geq s^2 C \frac{2}{2}$$

Therefore, by Lemma 5, with high probability

$$\Delta(R^{-+}) = -y^2 \sum_{j \in R^{-+}} v_j^2 \leq -\frac{x^2 s^2 C}{2}.$$  

We now bound from above the loss from false negatives. It is easy to verify that $\Delta(R^{++}) = x^2 \sum_{j \in R^{++}} b_j^2$. Let $\alpha = 4$, and denote $T = (s^2 n^2 \log n)/n$. Let $K = \{ j \mid b_j^2 \geq (4s^2 \alpha^2 \log n)/(c^2 n) \}$. By Lemma 2 and using the union bound, with high probability, for each $j \in R^+$ we have $v_j^2 \leq T$. By Lemma 3 and using the union bound, for each $j \in K$ with high probability $v_j^2 \geq T$. Thus, with high probability $R^{-+} \cap K = \phi$. Thus

$$\Delta(R^{++}) \leq |R^{++}| \frac{4x^2 s^2 \alpha^2 \log n}{c^2 n} \leq \frac{4C_0 x^2 s^2 \alpha^2}{c^2},$$

using $t \leq (C_0 n)/\log n$. By Lemma 4, with high probability $c^2 \geq 1/2$, and thus

$$\Delta(R^{++}) \leq 8C_0 x^2 s^2 \alpha^2$$

Putting it all together, with high probability and for $C_0$ chosen to be a small enough constant

$$\Delta(R^{++}) + \Delta(R^{-+}) \leq x^2 s^2 \left(8C_0 \alpha^2 - \frac{C}{2}\right) < 0.$$  

\[ \square \]

9 Conclusion

ReFACTor is a simple and effective algorithm for the recovery of low-rank matrices, which are suspected of column-sparsity, in the presence of noise. ReFACTor is very simple to implement and indeed is not more complicated than SVD or PCA. We have proved that ReFACTor is safe to use, in the sense that it offers equal or better performance compared to the baseline TSVD algorithm. Under mild conditions, the performance improvement over TSVD is provably significant. We have proven similar results for the variant ReFACTor+ (see Supporting Information). We note that the ReFACTor+ variant is critically important in practice, since it is not affected by scaling of the columns. We further presented extensive empirical evidence, under a very wide variety of conditions, that ReFACTor offers improved performance, sometimes significantly, over both the baseline TSVD and the algorithm of [14]. Finally, we have shown that ReFACTor provides scientific value in analysis of DNA methylation studies.

There are numerous important aspects, pertaining to the theoretical analysis of ReFACTor as well as to its implementation in the field, which this brief paper does not cover. For example, the empirical evidence
we present decisively suggest that our main results hold for $r > 1$ and $t > n / \log n$; this remains to be shown. Empirical evidence also decisively suggest that the performance of ReFACTor is very similar to that of ReFACTor∗; this also remains to be formally analyzed. Importantly, space did not allow us to discuss estimation of the parameters $\sigma$, $t$, and $r$, all of which are needed in order to successfully implement ReFACTor in practice.

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