A Bias Trick for Centered Robust Principal Component Analysis

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Abstract
Outlier based Robust Principal Component Analysis (RPCA) requires centering of the non-outliers. We show a “bias trick” that automatically centers these non-outliers. Using this bias trick we obtain the first RPCA algorithm that is optimal with respect to centering.

1 Introduction
Principal Component Analysis (PCA) is arguably the most widely used dimension reduction technique. It is known that the PCA model is heavily influenced by data outliers. The detection and removal of such outliers is a key component of robust variants of the PCA.

There are two main variants of standard PCA: centered and uncentered. The only difference between them is that in centered PCA there is a preliminary step where the data is being centered. From a computational point of view, there is little difference between these variants. For this reason, most recently published fast algorithms for computing PCA ignore the centering of the data. The situation is very different for algorithms that attempt to compute RPCA by identifying some points as outliers to be removed. The problem is that the centering should be applied only to the non-outliers, but they are unknown.

Some previously proposed RPCA algorithms perform initial centering of the data but do not update the center based on the outliers. These include (Zhang et al. 2015; Xu, Caramanis, and Sanghavi 2010; Shah et al. 2017). Other algorithms such as (Xu, Caramanis, and Mannor 2013; Rahmani and Atia 2017) do not explicitly center the data. The first assumes a probability distribution of the mean, and the second considers only directions of vectors which makes centering unnecessary. Other algorithms such as (Hubert and Engelen 2004) handle the centering as part of the algorithm, but not optimally. This review of the current state of the art suggests that optimal centering in RPCA is not fully solved.

We propose a general method (a bias trick) that can be used to convert any robust algorithm that does not perform centering into an algorithm that performs centering optimally. In fact, the bias trick can be used to convert any algorithm that computes uncentered PCA into an algorithm that computes a centered PCA.

Using the bias trick with the algorithm of (Shah et al. 2017) that computes optimal uncentered RPCA gives the first optimal centered RPCA algorithm. We implemented this algorithm and describe some experimental results, showing improved performance over all competitors.

2 The Bias Trick
Let PCA() be an uncentered PCA algorithm. It gets as input the matrix $X$ of size $m \times n$ and the number $k$ of desired principal vectors. It returns the principal vectors as the matrix $V$ of size $m \times k$, and $k$ eigenvalues. To apply the bias trick and obtain the centered PCA we do the following:

1. Select a large value $b$. (See Section 3)
2. Add $b$ as an additional coordinate to each column of $X$, creating a new matrix $X_b$ of size $(m+1) \times n$.
3. Run PCA() on $X_b$ to compute $k+1$ eigenvectors and eigenvalues. Each eigenvector is of size $(m+1)$.
4. Let $\lambda^b_1 \ldots \lambda^b_{k+1}$ be the eigenvalues computed in Step 3. Then the $k$ eigenvalues of the centered PCA are approximately $\lambda^b_2 \ldots \lambda^b_{k+1}$.
5. Let $u^b_1 \ldots u^b_{k+1}$ be the eigenvectors computed in Step 3. Let $v^b_j$ be the $j$th eigenvector of the centered PCA. It is given approximately by the top $m$ values of the $u^b_{k+1}$.

Clearly, the bias trick is not an improvement over the standard centered PCA algorithm. It is more costly and less accurate. But, it has the advantage that it also works for centered RPCA where it does not require advanced knowledge of the outliers. Applying the bias trick for computing centered RPCA can be achieved by using RPCA() instead of PCA(), where RPCA() is any uncentered RPCA algorithm.

3 Correctness of the Bias Trick
The following theorem is proved as a corollary in the Appendix.
Theorem: Let $X$ be the data matrix and let $\mu$ be the mean of $X$ columns. For any desired accuracy of computing the centered PCA of $X$ there exists $0<\epsilon<1$ such that setting $b\geq \sqrt{1-\epsilon^2}/\|\mu\|$ in the procedure outlined in Section 2 gives the desired approximation.

4 Experiments

In the first experiment, we demonstrate that centered PCA implemented with the bias trick returns accurate eigenvalues and eigenvectors. The error for the iris data (from UC Irvine) with various $\epsilon$ values is shown in Figure 1. Observe that for moderate values of $\epsilon$ and $b$ the error is almost 0. Similar results were obtained with other datasets, suggesting that $\epsilon\approx 0.2$, or $b\approx 5\|\mu\|$, may give sufficient accuracy.

Optimal Centered Robust PCA. We describe the results of using the algorithm of (Shah et al. 2017) with the bias trick. The original algorithm computes optimal uncentered RPCA. With the bias trick the algorithm computes optimal centered RPCA. To the best of our knowledge this is the first centered algorithm with guaranteed optimality. We refer to this algorithm as COPT.

Tables 1, 2 show errors for several algorithms using code provided by the authors. The values are the average reconstruction error of the $n$ non-outlier points: $E_{\text{rpca}} = \frac{1}{n} \sum_{i=1}^{n} ||x_i - \mu||^2 - V_{\text{rpca}} V_{\text{rpca}}^T (x_i - \mu)||^2$. Our COPT is clearly superior.

Figures 2, 3 compare the results of our COPT algorithm to the results of the Outlier-Pursuit algorithm. Five outliers were selected based on the first two principal vectors. The left panel in both figures shows the location of points in the plane defined by these vectors. The right panel is the location of points on the plane defined by the first and third principal vectors. The horizontal line is the plane composed of the first two principal vectors. Indeed, the locations of outliers are far away from the locations of non-outliers in the third principal vector direction. As shown on the right panel in Figure 2, the five selected outliers are the furthest ones away from the horizontal line. In Figure 3 the outliers are not the ones farthest away especially for the points 69 and 95. This illustrates that our COPT returns better outliers than Outlier-Pursuit algorithm.
Appendix: correctness of the bias trick

In this appendix we prove the correctness of the bias trick. An important part can be traced back to Cadima and Jolliffe 2009. In that paper they prove the following result (as a corollary to their Theorem 2).

**Theorem:** (Cadima and Jolliffe): Let $B$ be the matrix of second moments of the centered data, let $\mu$ be the data mean, and let $C$ be the covariance matrix. If one of the eigenvectors of $B$ is $\mu/\|\mu\|$ then all other eigenvector/eigenvalue pairs of $B$ are also eigenvector/eigenvalue pairs of $C$.

**Notation**

Let $X = (x_1 \ldots x_n)$ be the data matrix, let $\mu = \frac{1}{n} \sum_i x_i$ be the data mean, and let $B = \frac{1}{n} \sum_i x_i x_i^T$ be the data second moments matrix. The covariance matrix is given by: $C = \frac{1}{n} \sum_i (x_i - \mu)(x_i - \mu)^T$. Let $\lambda_i, v_i$ be the eigenvalue/eigenvector pairs of $C$.

Create $X_b = (x_1^b \ldots x_n^b)$ by adding a large bias $b$ for each vector: $x_i^b = \frac{x_i}{b}$. $X_b$ is $(m+1)\times n$. The column mean of $X_b$ is: $\mu_b = \frac{\mu}{b}$. The corresponding $(m+1)\times(m+1)$ matrix of second moments is:

$$B_b = \frac{1}{n} \sum_i x_i^b (x_i^b)^T = \left( B \begin{bmatrix} b & \mu \end{bmatrix} \begin{bmatrix} b & \mu \end{bmatrix} \right)$$

and the corresponding covariance matrix is:

$$C_b = \frac{1}{n} \sum_i (x_i^b - \mu_b) (x_i^b - \mu_b)^T = \begin{bmatrix} C & 0 \\ 0 & 0 \end{bmatrix}$$

Let $\lambda_i^b, v_i^b$ be the eigenvalue/eigenvector pairs of $B_b$. Define: $v_i = \frac{v_i^b}{b}$, where $v_i$ is an $m$-vector and $b$ is a scalar. The bias trick is useful since (as proved here) $u_i \approx v_{i+1}$ and $\lambda_i \approx \lambda_{i+1}$. Thus, the centered eigenvectors and eigenvalues are obtained from the uncentered and “biased” eigenvectors and eigenvalues.

To analyze the bias trick we need the notion of “approximation for sufficiently large values of the bias $b$”. It is defined as follows:

**Definition:** We write $p \approx q$ if for any $\epsilon > 0$ there is $b_\epsilon$ such that $(p - q)^2 < \epsilon$ for all $b > b_\epsilon$. When $p, q$ are vectors the squared error is replaced with squared norm, etc. We also say “$p$ approximates $q$” if $p \approx q$.

**Lemma 1.** For a sufficiently large value of $b$:

Part 1. $w_1 \approx \frac{b}{\sqrt{b^2 + \|\mu\|^2}}$ Part 2. $v_1 \approx \frac{\mu}{\sqrt{b^2 + \|\mu\|^2}}$

**Proof:** From the Courant Fischer theorem (Golub and Van-Loan 2013) the vector $v_1$ and the scalar $w_1$ minimize the following error:

$$E(v_1, w_1) = \min_{a_i} \sum_i \|x_i - a_i v_1\|^2 = \min_{a_i} \sum_i \|x_i - a_i v_1\|^2 + (b - a_i w_1)^2$$

For sufficiently large value of $b$ the rightmost term dominates the error and it is minimized by $a_i = \frac{b}{w_1}$. Substituting this in (2) gives: $E(v_1, w_1) = \sum_i \|x_i - \frac{b}{w_1} v_1\|^2$. Since $v_1$ and $w_1$ form an eigenvector they must satisfy: $|v_1|^2 + w_1^2 = 1$. To minimize $E(v_1, w_1)$ subject to this constraint we use the method of Lagrange multipliers. The Lagrangian is:

$$L(v_1, w_1, \alpha) = \sum_i \|x_i - \frac{b}{w_1} v_1\|^2 + \alpha(v_1^2 + w_1^2 - 1)$$

Taking derivatives of (3) with respect to $v_1$ and equating to 0 gives: $(-b/w_1)(n\mu - \frac{b}{w_1} v_1) + 2\alpha v_1 = 0$. Therefore, the vectors $v_1$ and $\mu$ are linearly dependent: $v_1 = t\mu$. Substituting this in the constraint and solving for $t$ we get: $t = \frac{\sqrt{1 - w_1^2}}{|\mu|}$.

$$v_1 \approx \frac{\sqrt{1 - w_1^2}}{|\mu|} \mu$$

To prove Part 1 we take derivatives of (3) with respect to $w_1$ and equate to 0. This gives:

$$2b v_1^T \mu / w_1^2 - 2nb^2 |v_1|^2 / w_1^3 + 2\alpha w_1 = 0$$

For sufficiently large $b$ the right most term can be ignored. After multiplying by $w_1^2$ and simplifying this gives:

$$w_1 v_1^T \mu \approx b |v_1|^2$$

Substituting the value of $v_1$ from (4) we get the following equation in $w_1$:

$$w_1 \|\mu\| \approx b \sqrt{1 - w_1^2}$$

Solving this equation for $w_1$ gives the formula in Part 1. Substituting the Part 1 expression for $w_1$ in (4) and simplifying gives the formula in Part 2.

**Theorem 1.** For a sufficiently large value of $b$ let $\lambda_i^b, v_i^b$ be an eigenvalue/eigenvector pair of $B_b$ with $i > 1$. Suppose $u_i^b$ is partitioned as follows: $u_i^b = \begin{bmatrix} v_i^b \\ w_i^b \end{bmatrix}$. Then $w_i \approx 0$ and $\lambda_i, v_i$ are approximately eigenvalue/eigenvector pairs of $C_b$.

**Proof:** From Lemma 1 it follows that

$$\begin{bmatrix} v_1 \\ b \end{bmatrix} \approx \frac{\mu_b}{\|\mu_b\|}$$

Since this approximately satisfies the condition of the Cadima and Jolliffe theorem stated above it follows that all other eigenvector/eigenvalue pairs of $B_b$ are also approximately eigenvector/eigenvalue pairs of $C_b$. From (1) it follows that if $z$ is the $m+1$ vector $\begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$ where $z_1$ is an $m$-vector and $z_2$ is a scalar then $C_b z = \begin{bmatrix} C z_1 \\ 0 \end{bmatrix}$. Therefore, if $C_b z = \lambda z$ then $z_2 = 0$ and $C z_1 = \lambda z_1$. 


Corollary. The sufficiently large value of \( b \) in Theorem 1 can be selected as:

\[
b \geq \frac{\sqrt{1-\epsilon^2}}{\epsilon \|\mu\|}
\]

for sufficiently small value of \( \epsilon \), where \( 0 \leq \epsilon \leq 1 \).

Proof: Set \( \epsilon = \sqrt{1-w_1^2} \). Substituting this value in Part 1 of Lemma 1 and solving for \( b \) gives the above relation. ■

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