Distributed Estimation for Principal Component Analysis: a Gap-free Approach

Xi Chen*1, Jason D. Lee†2, He Li‡1, and Yun Yang§3

1Stern School of Business, New York University
2Department of Electrical Engineering, Princeton University
3Department of Statistics, University of Illinois at Urbana-Champaign

Abstract

The growing size of modern data sets brings many challenges to the existing statistical estimation approaches, which calls for new distributed methodologies. This paper studies distributed estimation for a fundamental statistical machine learning problem, principal component analysis (PCA). Despite the massive literature on top eigenvector estimation, much less is presented for the top-$L$-dim ($L > 1$) eigenspace estimation, especially in a distributed manner. We propose a novel multi-round algorithm for constructing top-$L$-dim eigenspace for distributed data. Our algorithm takes advantage of shift-and-invert preconditioning and convex optimization. Our estimator is communication-efficient and achieves a fast convergence rate. In contrast to the existing divide-and-conquer algorithm, our approach has no restriction on the number of machines. Theoretically, we establish a gap-free error bound and abandon the assumption on the sharp eigengap between the $L$-th and the $(L + 1)$-th eigenvalues. Our distributed algorithm can be applied to a wide range of statistical problems.

*e-mail: xchen3@stern.nyu.edu. Xi Chen would like to thank the support from NSF via IIS-1845444.
†e-mail: jasonlee@princeton.edu.
‡e-mail: hli@stern.nyu.edu.
§e-mail: yy84@illinois.edu.
based on PCA. In particular, this paper illustrates two important applications, principal component regression and single index model, where our distributed algorithm can be extended. Finally, We provide simulation studies to demonstrate the performance of the proposed distributed estimator.

**Keywords:** Distributed estimation, Principal component analysis, Shift-and-invert preconditioning, Gap-free convergence analysis

1 Introduction

The development of technology has led to the explosive growth in the size of modern data sets. The challenge arises, when memory constraints and computation restrictions make the traditional statistical estimation and inference methods no longer applicable. For example, in a sensor network, the data are collected on each tensor in a distributed manner. The communication cost would be rather high if all the data are transferred and computed on a single (central) machine, and it may be even impossible for the central machine to store and process computation on such large-scale datasets. Distributed statistical approaches have drawn a lot of attentions these days and methods are developed for various statistics problems, such as sparse regression (see, e.g., Lee et al. (2017)), likelihood-based inference (see, e.g., Battey et al. (2018); Jordan et al. (2019)), kernel ridge regression (Zhang et al., 2015), semi-parametric partial linear models (Zhao et al., 2016), quantile regression (see, e.g., Volgushev et al. (2019); Chen et al. (2019)), linear support vector machine (Wang et al., 2019), and $M$-estimators with cubic rate (Shi et al., 2018; Banerjee et al., 2019). All these works are seeking for distributed statistical methods that are able to handle massive computation tasks efficiently for large-scale data and achieve the same convergence rate as those classical methods as well.
In a typical distributed environment, each machine has access to a different subset of samples of the whole data set. The communication and computation follow from a hierarchical master-slave-type architecture, where a central machine acts as a fusion node. Computation tasks for local machines and the central machine are different. After local machines finish their computation, the local results will be transferred to the master machine, where they will be merged together and the fusioned result will be transferred back to all local machines for the next step.

In this paper, we study the problem of principal component analysis (PCA) in a distributed environment. PCA (Pearson, 1901; Hotelling, 1933) is one of the most important and fundamental tools in statistical machine learning. For random vectors $a_1, \ldots, a_n$ in $\mathbb{R}^d$ with mean zero and covariance matrix $\Sigma$, its empirical covariance matrix is $\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} a_i a_i^\top$. The $L$-PCA ($L \leq d$) finds a $L$-dimension subspace projection that preserves the most variation in the data set, which is equivalent to the following optimization problem:

$$\max_{U \in \mathbb{R}^{d \times L}: U^T U = I_L} \left\| \hat{\Sigma} U \right\|_F,$$

where $\left\| \cdot \right\|_F$ denotes the matrix Frobenius norm and $I_L$ is the $L \times L$ identity matrix. In other words, $U \in \mathbb{R}^{d \times L}$ is the top-$L$-dim eigenspace of $\hat{\Sigma}$. PCA has been widely used in many aspects of statistical machine learning, e.g., principal component regression (Jeffers, 1967; Jolliffe, 1982), single index model (Li, 1992), representation learning (Bengio et al., 2013).

Under distributed regime, Fan et al. (2019) proposed a novel one-shot type of algorithm which is often called divide-and-conquer (DC) method. In Fan et al. (2019), DC method first computes local covariance matrices $\hat{\Sigma}_i$ on each machine $k = 1, \ldots, K$. Eigenspaces $\hat{U}_k, k = 1, \ldots, K$ are then computed locally using the traditional PCA algorithm and transmitted to the central machine. Central machine combines local eigenspaces $\hat{U}_k$ into an aggregated
covariance estimator, \( \tilde{\Sigma} = \frac{1}{K} \sum_{k=1}^{K} \hat{U}_k \hat{U}_k^\top \). The final estimator is obtained as the top-\( L \)-dim eigenspace of \( \tilde{\Sigma} \). DC method is easy to implement and requires only \( O(dL) \) communications for each local machine, where \( d \) denotes the data dimension, \( n \) the total sample size, and \( m \) the sample size on each local machine. Let us denote the condition number of the population covariance matrix \( \Sigma \) by \( \rho \), i.e., \( \rho = \lambda_1/(\lambda_L - \lambda_{L+1}) \), and the effective rank of \( \Sigma \) by \( r = \text{Tr}(\Sigma)/\lambda_1 \). For asymmetric innovation distributions, Fan et al. (2019) showed that when the number of machines is not very large (no greater than \( O(m/(\rho^2 r)) \)), DC method enjoys a optimal statistical convergence rate of order \( O(\rho \sqrt{Lr/n}) \). However, when the number of machines becomes larger, DC method only achieves a slow convergence rate of \( O(\rho \sqrt{Lr/n} + \rho^2 \sqrt{Lr/m}) \). This feature may not be desirable in distributed settings. For example, in a sensor network with a vast number of sensors, the number of machines may exceed the constraint set for the optimal rate. The precise definition of asymmetric innovation above is given in Section 4.2 of Fan et al. (2019). Roughly speaking, a random variable \( a \in \mathbb{R}^d \) is distributed under asymmetric innovation if flipping the sign of one component of \( a \) changes its distribution.

One question naturally arises from the analysis of DC method, can we possibly relax the restriction on the number of machines? Motivated by this question, our paper presents a multi-round distributed algorithm for top-\( L \)-dim eigenspace estimation. As compared to DC method in Fan et al. (2019), we completely remove the assumption on the number of machines. Our method leverages shift-and-invert preconditioning (a.k.a., Rayleigh quotient iteration) from numerical analysis (Van Loan and Golub, 2012) together with quadratic programming and achieves a fast convergence rate. Moreover, many previous convergence analysis of eigenspace estimation also relies on the assumption of a sharp eigengap between the \( L \)-th and the \((L + 1)\)-th eigenvalues \( \lambda_L \) and \( \lambda_{L+1} \), i.e., \( \lambda_L - \lambda_{L+1} > 0 \), or other specific
eigen-structures of $\Sigma$. Here, in our theoretical part, we drop this eigengap assumption and present a gap-free type result.

The idea of solving PCA via shift-and-invert preconditioning has long history in numerical analysis (Van Loan and Golub, 2012). It is an iterative method that sequentially solves linear system to obtain increasingly accurate eigenvector estimates. Its connection with convex optimization has been studied in the past decade. In a single-machine setting, Garber et al. (2016); Allen-Zhu and Li (2016) formulate each round of shift-and-invert preconditioning as a quadratic optimization problem and it can be solved with first-order deterministic (accelerated) gradient method like Nestrov accelerated method. Garber and Hazan (2015); Shamir (2016); Xu (2018) also relate the same convex optimization problem with variance-reduction stochastic technique (SVRG, see, e.g.,, Johnson and Zhang (2013)). Furthermore, in distributed settings, Garber et al. (2017) perform a multi-round algorithm but they only consider the estimation task of the first eigenvector. This paper proposes a general distributed algorithm that estimates the top-$L$-dim eigenspace without any restriction on the eigengap.

The proposed algorithm can facilitate many fundamental applications based on PCA in distributed environment. In particular, we illustrate two important applications, namely principal component regression (see Section 4.1) and single index model (see Section 4.2).

**Example 1: principal component regression**

Introduced by Jeffers (1967); Jolliffe (1982), principal component regression (PCR) is a regression analysis technique based on PCA. Typically, PCR assumes a linear model $y = A\beta^* + \epsilon$ with the further assumption that coefficient $\beta^*$ lies in the low-rank eigenspace of data covariance matrix. Therefore, PCA can be performed to obtain the principal components
\( \hat{U}_L \) of the observed covariance matrix \( \hat{\Sigma} = \frac{1}{n} A^\top A \) and the data matrix \( A \) is then projected on \( \hat{U}_L \). The estimator \( \hat{\beta} \) of \( \beta^* \) is then obtained by regress \( y \) on this projected data matrix \( A\hat{U}_L \). Many previous work has analyze the statistical property of PCR, see Frank and Friedman (1993); Bair et al. (2006). Under a distributed environment, our distributed PCA algorithm can replace the traditional PCA algorithm in the above procedure and lead to a distributed algorithm for PCR. As we will show in Section 4.1, this distributed estimator achieves a similar error as in the single-machine setting.

**Example 2: single index model**

Single index model (Li, 1992) considers a semi-parametric regression model \( y = f(\langle \beta^*, a \rangle) + \epsilon \). Under some mild condition on the link function \( f(\cdot) \), we would like to make estimation on the coefficient \( \beta^* \) using observed data \( \{a_i, y_i\}_{i=1}^n \) without knowing \( f(\cdot) \). Some previous methods include semi-parametric maximum likelihood estimator (Horowitz, 2009) and gradient-based estimator (Hristache et al., 2001). Moreover, many works propose to use Stein’s identity (Stein, 1981; Janzamin et al., 2014) to estimate \( \beta^* \) (see, e.g., Li (1992); Yang et al. (2017) and references therein). Specifically, under Gaussian innovation where \( a \) is standard multivariate normal random vector, the estimator \( \hat{\beta} \) can be calculated from the top eigenvector of \( \frac{1}{n} \sum_{i=1}^n y_i \cdot (a_i a_i^\top - I_d) \). This method can be naturally extended to a distributed manner with a distributed eigen-decomposition of \( \frac{1}{n} \sum_{i=1}^n y_i \cdot (a_i a_i^\top - I_d) \).

### 1.1 Notations

We first introduce the notations related to our work. We write vectors in \( \mathbb{R}^d \) in boldface lower-case letters (e.g., \( a \)), matrices in boldface upper-case letters (e.g., \( A \)), and scalars are written in lightface letters (e.g., \( t \)). Let \( \| \cdot \| \) denote vector norm (e.g., \( \| \cdot \|_2 \) is standard
Euclidean norm for vectors). Matrix norm is written as $\|\cdot\|$. For a matrix $A \in \mathbb{R}^{n \times d}$, $\|A\|_2$ and $\|A\|_F$ represent the spectral norm and Frobenius norm respectively. Furthermore, $0$ represents zero vector with corresponding dimension and identity matrix with dimension $d \times d$ is shortened as $I_d$. We use $e_1, \ldots, e_d$ to denote the standard unit vectors in $\mathbb{R}^d$, i.e., $e_i = [0, \ldots, 0, 1, 0, \ldots, 0]$ where only the $i$-th element of $e_i$ is 1.

We use $\mathcal{O}_p$ to describe a high probability bound with constant term omitted. We also use $\tilde{\mathcal{O}}_p$ to further omit the logarithm factors.

We adopt the standard definition of sub-Gaussian random vectors (see, e.g., Vershynin (2012); Rigollet and Hütter (2015)) that a random vector $a \in \mathbb{R}^d$ is said to be a $d$-dimensional sub-Gaussian with variance proxy $\sigma$ if $E[a] = 0$ and for any unit vector $u$,

$$
E[\exp(s a^\top u)] \leq \exp \left( \frac{\sigma^2 s^2}{2} \right), \forall s \in \mathbb{R}.
$$

1.2 Paper organization

The remainder of this paper is organized as follows. In Section 2, we introduce the problem setups of the distributed PCA and give our algorithms. Section 3 develops the convergence analysis of our estimator. Two application scenarios, i.e., principal component regression and single index model are introduced in Section 4 where we provide convergence analysis for both single-machine and distributed settings. Finally, extensive numerical experiments are provided in Section 5. The technical proofs and some additional experimental results are provided in the supplementary material.
2 Problem Setsups

In the following section, we collect the setups for our distributed PCA and present the algorithms.

Assume that there are \( n \) i.i.d. zero mean vectors \( \mathbf{a}_i \) sampling from some distribution \( \mathcal{D} \) in \( \mathbb{R}^d \). Let \( \mathbf{A} = [\mathbf{a}_1, \ldots, \mathbf{a}_n]^\top \in \mathbb{R}^{n \times d} \) be the data matrix. Let \( \Sigma \) be the population covariance matrix \( \Sigma = \mathbb{E}_{\mathbf{a} \sim \mathcal{D}} [\mathbf{a} \mathbf{a}^\top] \) with the eigenvalues \( \lambda_1(\Sigma) \geq \lambda_2(\Sigma) \geq \ldots \lambda_d(\Sigma) \geq 0 \) and the associated eigenvectors are \( \mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_d] \in \mathbb{R}^{d \times d} \).

In the distributed principal component analysis, for a given number \( L, 1 \leq L \leq d \), we are interested in estimating the eigenspace spanned by \( \{\mathbf{u}_1, \ldots, \mathbf{u}_L\} \) in a distributed environment. We assume \( n \) samples are split uniformly at random on \( K \) machines, where each machine contains \( m \) samples, i.e., \( n = mK \). We note that since our algorithm aggregates gradient information across machines, it can handle the unbalanced data case without any modification. We choose to present the balanced data case only for the ease of presentation (see Remark 3.8 for more details). The data matrix on each machine \( k \) is denoted by \( \mathbf{A}_k \in \mathbb{R}^{m \times d} \) for \( k = 1, \ldots K \).

Let us first discuss a special case (illustrated in Algorithm 1), where we estimate the top eigenvector, i.e., \( L = 1 \). The basic idea of our Algorithm 1 is as follows.

Let \( \mathbf{w}^{(0)} \) be the initial estimator of the top eigenvector and \( \bar{\lambda}_1 \) a crude estimator of an upper bound of the top eigenvalue. Here we propose to compute \( \mathbf{w}^{(0)} \) and \( \bar{\lambda}_1 \) only using the data from the first machine, and thus there does not incur any communication cost. For example, \( \bar{\lambda}_1 \) can be computed with \( \bar{\lambda}_1 = \lambda_1(\mathbf{A}_1^\top \mathbf{A}_1/m) + 3\eta/2 \), where \( \lambda_1(\mathbf{A}_1^\top \mathbf{A}_1/m) \) is the top eigenvalue for the empirical covariance matrix on the first machine and \( \eta \) is a special constant defined later in Equation (9). The \( \mathbf{w}^{(0)} \) can be simply computed via eigenvalue
Algorithm 1 Distributed Top Eigenvector (Distri-Eigen)

**Input:** Data matrix $A_k$ on each machine $k = 1, \ldots, K$. The initial top eigenvalue estimator $\lambda_1$ and eigenvector estimator $w^{(0)}$. The number of outer iterations $T$ and the number of inner iterations $T'$.

1: Distribute $\lambda_1$ to each local machine and each local machine computes $H_k = \lambda_1 I - A_k^\top A_k/m$.

2: for $t = 0, 1, \ldots, (T - 1)$ do

3: Distribute $w^{(t)}$ to each local machine and each local machine sets $w_0^{(t+1)} = w^{(t)}$

4: for $j = 0, 1, \ldots, (T' - 1)$ do

5: for each local machine $k = 1, \ldots, K$ do

6: Compute the local gradient information $g_k = H_k w_j^{(t+1)} - w^{(t)}$

7: Transmit the local gradient information $g_k$ to the central machine.

8: end for

9: Calculate the global gradient information $g = \frac{1}{K} \sum_{k=1}^{K} g_k$.

10: Perform the approximate Newton’s step: $w_j^{(t+1)} = w_j^{(t+1)} - H_1^{-1} g$.

11: end for

12: end for

13: The central machine updates $w^{(t+1)} = \frac{w_j^{(t+1)}}{\|w_j^{(t+1)}\|_2}$.

14: Output: $w^{(T)}$.

decomposition of $A_1^\top A_1/m$.

Given $w^{(0)}$ and $\lambda_1$, we perform the *shift-and-invert preconditioning* iteration in a distributed manner. In particular, for each iteration $t = 0, 1, \ldots,$

$$\tilde{w}^{(t+1)} = \left(\lambda_1 I - \frac{1}{n} A_1^\top A_1\right)^{-1} w^{(t)},$$

$$w^{(t+1)} = \frac{\tilde{w}^{(t+1)}}{\|\tilde{w}^{(t+1)}\|_2}.$$  

Therefore, the non-convex eigenvector estimation problem (1) is reduced to solving a sequence of linear system. The key challenge is how to implement $\left(\lambda_1 I - A_1^\top A_1/n\right)^{-1}$ in a
To address this challenge, we formulate (2) into a quadratic optimization problem. In particular, the update \( \tilde{w}^{(t+1)} = (\lambda_1 I - A^TA/n)^{-1}w^{(t)} \) is equivalent to the following problem,

\[
\tilde{w}^{(t+1)} = \arg \min_w \left[ Q(w) := \frac{1}{2} w^T H w - w^T w^{(t)} \right], \tag{3}
\]

\[ H \triangleq \lambda_1 I - \frac{1}{n} A^TA. \]

To solve this quadratic programming, the standard Newton’s approach computes a sequence for \( j = 0, \ldots \), with a starting point \( w_0^{(t+1)} = w^{(t)} \):

\[
w_{j+1}^{(t+1)} = w_j^{(t+1)} - \left( \nabla^2 Q(w_j^{(t+1)}) \right)^{-1} \left[ \nabla Q(w_j^{(t+1)}) \right], \tag{4}
\]

where the Hessian matrix \( \nabla^2 Q(w_j^{(t+1)}) \) is indeed \( H \). If we define, for each machine \( k = 1, \ldots, K \),

\[
H_k = \lambda_1 I - \frac{1}{m} A_k^T A_k, \tag{5}
\]

\[
Q_k(w) = \frac{1}{2} w^T H_k w - w^T w^{(t)}. \]

It is easy to see that \( H = \sum_{k=1}^K H_k / K \) and \( Q(w) = \sum_{k=1}^K Q_k(w) / K \). Therefore, in the Newton’s update (4), computing the full Hessian matrix \( \nabla^2 Q(w_j^{(t+1)}) \) requires each machine to communicate a \( d \times d \) local Hessian matrix \( H_k \) to the central machine. This procedure incurs a lot of communication cost. Moreover, taking the inverse of the whole sample Hessian matrix \( H \) almost solves the original linear system (2). To address this challenge, we adopt the idea from Shamir et al. (2014); Jordan et al. (2019); Fan et al. (2019). In particular, we approximate the Newton’s iterates by only using the Hessian information on the first machine, which significantly reduces the communication cost. This approximated Newton’s update can be written as,
\[
\begin{align*}
\mathbf{w}_{j+1}^{(t+1)} &= \mathbf{w}_j^{(t+1)} - \left(\nabla^2 Q_1(\mathbf{w}_j^{(t+1)})\right)^{-1} \left[\nabla Q(\mathbf{w}_j^{(t+1)})\right] \\
&= \mathbf{w}_j^{(t+1)} - \mathbf{H}_1^{-1} \left[\frac{1}{K} \sum_{k=1}^{K} (\mathbf{H}_k \mathbf{w}_j^{(t+1)} - \mathbf{w}^{(t)})\right],
\end{align*}
\]

where \(\mathbf{H}_1\) is the Hessian matrix of the first machine. This procedure can be computed easily in a distributed manner, i.e., each machine computes local gradient \(\mathbf{g}_k = \mathbf{H}_k \mathbf{w}_j^{(t+1)} - \mathbf{w}^{(t)}\), and these gradient vectors are communicated to the central machine for a final update \(\mathbf{g} = \sum_{k=1}^{K} \mathbf{g}_k / K\). Therefore, in each inner iteration, the communication cost for each local node is only \(O(d)\). See Algorithm 1 for a complete description.

For the top-\(L\)-dim eigenspace estimation, we extend a framework from Allen-Zhu and Li (2016) to our distributed settings. In our Algorithm 2, we first compute the leading eigenvector \(\mathbf{v}_1\) of \(\mathbf{A}^\top \mathbf{A}/n\) in a distributed manner with Algorithm 1. The \(\mathbf{v}_1\) is then transferred back to local machines and used to right-project data matrix, i.e., \(\mathbf{A}_k(\mathbf{I}_d - \mathbf{v}_1 \mathbf{v}_1^\top)\) for \(k = 1, \ldots, K\). The next eigenvector \(\mathbf{v}_2\) is obtained with these projected data matrices and Algorithm 1. In other words, we estimate the top eigenvector of \((\mathbf{I}_d - \mathbf{v}_1 \mathbf{v}_1^\top) \hat{\mathbf{\Sigma}} (\mathbf{I}_d - \mathbf{v}_1 \mathbf{v}_1^\top)\) in distributed settings. This procedure is repeated \(L\) times until we obtain all the \(L\) top eigenvectors \(\mathbf{V}_L = [\mathbf{v}_1, \ldots, \mathbf{v}_L]\). This deflation technique is quite straight-forward and performs well in our later convergence analysis.

## 3 Theoretical Properties

This section exhibits the theoretical results for our setups in Section 2. We provide proofs in the supplement.
Algorithm 2 Distributed Top-$L$-dim principal subspace

**Input:** The data matrix $A_k$ on each machine $k = 1, \ldots, K$. The number of top-eigenvectors $L$.

1: Initialize $V_0 = [], A_{k,0} = A_k$
2: for $l = 1, \ldots, L$ do
3: Compute the initial $l$-th eigenvalue estimator $\hat{\lambda}_l$ and eigenvector estimator $w_l^{(0)}$.
4: Call Algorithm 1 with $\{A_{k,l-1}\}_{k=1}^K$ on each local machine to obtain $w_l$ on the central machine.
5: Project $w_l$ to $V_{l-1}^\perp$ by computing $v_l = \frac{(I-V_{l-1}V_{l-1}^\top)w_l}{\| (I-V_{l-1}V_{l-1}^\top)w_l \|_2}$ as the estimated $l$-th eigenvector
6: Update $V_l = [V_{l-1}, v_l]$
7: Transmit $v_l$ to each local machine.
8: for each local machine $k = 1, \ldots, K$ do
9: Update the data matrix $A_{k,l} = A_{k,l-1}(I - v_lv_l^\top)$
10: end for
11: end for
12: Output: $V_L$. 

### 3.1 Distributed top eigenvector estimation

We first investigate the theoretical properties of the top eigenvector estimation in Algorithm 1. Let $\hat{\Sigma}_k = A_k^\top A_k/m \in \mathbb{R}^{d \times d}$ denote the local sample covariance matrix on machine $k = 1, \ldots, K$, and $\hat{\Sigma} = K^{-1}\sum_{k=1}^K \hat{\Sigma}_k$ the global sample covariance matrix using all data. Let $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \cdots \geq \hat{\lambda}_d \geq 0$ and $\hat{u}_1, \hat{u}_2, \ldots, \hat{u}_d$ denote the sorted eigenvalues and associated eigenvectors of $\hat{\Sigma}$. We are interested in eigenvalue gap-free type results. More specifically, we will reserve the letter $\delta$ to denote the relative eigenvalue gap threshold, and will measure the closeness between $w^{(t)}$ and the top eigenvector $\hat{u}_1$ via proving

$$\sum_{l: \hat{\lambda}_l \leq (1-\delta)\hat{\lambda}_1} |\langle \hat{u}_l, w^{(t)} \rangle|^2 \leq \frac{\varepsilon^2}{\delta^2},$$

(7)
for error $\varepsilon > 0$ and any constant $\delta \in (0, 1)$. In particular, such an eigenvalue gap-free bound (7) is always stronger (modulo constants) than the usual bound

$$\hat{\theta}(t) : = \arccos |\langle \hat{u}_1, w^{(t)} \rangle| \leq C \varepsilon \frac{\hat{\lambda}_1}{\lambda_1 - \hat{\lambda}_2},$$

that involves the relative gap between the first two eigenvalues of $\hat{\Sigma}$. Here $C$ is a constant.

To see this, we can simply choose $\delta = (\hat{\lambda}_1 - \hat{\lambda}_2)/\hat{\lambda}_1$ in the gap-free bound. Then $\sin^2 \hat{\theta}(t) = 1 - |\langle \hat{u}_1, w^{(t)} \rangle|^2 = \sum_l: \hat{\lambda}_l \leq (1 - \delta) \hat{\lambda}_1 |\langle \hat{u}_l, w^{(t)} \rangle|^2 \leq \varepsilon^2/\delta^2$, implying $\hat{\theta}(t) \leq \arcsin(\varepsilon/\delta) \leq C \varepsilon \hat{\lambda}_1/(\hat{\lambda}_1 - \hat{\lambda}_2)$ for some universal constant $C > 0$. Moreover, it has to be assumed that $\hat{\lambda}_1 > \hat{\lambda}_2$ in the usual bound (8), which may not be held in some applications.

As we will show in the theoretical analysis later, the success of our algorithm relies on the initial values of both eigenvalue and eigenvector. We first clarify our choice of initial eigenvalue estimates.

For the top eigenvector estimation in Algorithm 1, since we have the following high probability bound (see Equation (23) in Lemma 3.5 at the end of this section for the justification),

$$\|\hat{\Sigma} - \hat{\Sigma}_1\|_2 \leq \eta/2,$$

for some constant $\eta > 0$. If we choose $\bar{\lambda}_1 = \lambda_1(\hat{\Sigma}_1) + 3\eta/2$, then it is guaranteed that

$$2\eta \geq \bar{\lambda}_1 - \lambda_1 \geq \eta.$$

Lemma 3.5 (Equation (24)) also provides a gap-free concentration bound on our initial value of eigenvectors,

$$\sum_{l: \hat{\lambda}_l \leq (1 - \delta) \hat{\lambda}_1} |\langle \hat{u}_l, w^{(0)} \rangle|^2 \leq \frac{3}{4},$$

with high probability. Here $\{\hat{u}_l : \hat{\lambda}_l \leq (1 - \delta) \hat{\lambda}_1\}$ are all the eigenvectors for the full sample covariance matrix $\hat{\Sigma}$ whose associated eigenvalues have a relative gap $\delta$ from the largest
eigenvalue \( \hat{\lambda}_1 \) and \( \mathbf{w}^{(0)} \) is the top eigenvector for the sample covariance matrix on the first machine.

With the above guarantees of initial estimator \( \overline{\lambda}_1 \) and \( \mathbf{w}^{(0)} \) in (10) and (11), our first lemma characterizes the convergence rate of the outer loop in Algorithm 1.

**Lemma 3.1.** Suppose the initial estimator \( \overline{\lambda}_1 \) satisfies

\[
\eta \leq \overline{\lambda}_1 - \hat{\lambda}_1 \leq 2\eta \quad \text{for some } \eta > 0. \tag{12}
\]

For any \( \mathbf{w} \in \mathbb{R}^d \), and \( \mathbf{v} \in \mathbb{R}^d \) that satisfies

\[
\|\mathbf{w}\|_2 = 1, \quad \sum_{l: \hat{\lambda}_l \leq (1 - \delta) \overline{\lambda}_1} |\langle \hat{\mathbf{u}}_l, \mathbf{w} \rangle|^2 \leq \frac{3}{4}, \tag{13}
\]

and

\[
\|\mathbf{v} - \mathbf{H}^{-1}\mathbf{w}\|_2 \leq \varepsilon \leq (8\eta)^{-1}. \tag{14}
\]

Therefore, for each index \( l = 1, \ldots \) such that \( \hat{\lambda}_l \leq (1 - \delta) \overline{\lambda}_1 \), we have

\[
\frac{|\langle \hat{\mathbf{u}}_l, \mathbf{v} \rangle|}{\|\mathbf{v}\|_2} \leq \frac{8\eta}{\delta \overline{\lambda}_1} |\langle \hat{\mathbf{u}}_l, \mathbf{w} \rangle| + 8\eta \varepsilon. \tag{15}
\]

Moreover, we have

\[
\sum_{l: \hat{\lambda}_l \leq (1 - \delta) \overline{\lambda}_1} \frac{|\langle \hat{\mathbf{u}}_l, \mathbf{v} \rangle|^2}{\|\mathbf{v}\|_2^2} \leq \frac{128\eta^2}{\delta^2 \overline{\lambda}_1^2} \sum_{l: \hat{\lambda}_l \leq (1 - \delta) \overline{\lambda}_1} \frac{|\langle \hat{\mathbf{u}}_l, \mathbf{w} \rangle|^2}{\|\mathbf{w}\|_2^2} + 128\eta^2 \varepsilon^2. \tag{16}
\]

*Proof.* Deferred to Appendix A in the supplement. \( \Box \)

For the outer loop in our Algorithm 1, \( \mathbf{w} \) and \( \mathbf{v}/\|\mathbf{v}\|_2 \) in Lemma 3.1 can be explained as the \( t \)-th round and \( (t + 1) \)-th round estimators \( \mathbf{w}^{(t)} \) and \( \mathbf{w}^{(t+1)} \), respectively. This lemma implies that up to a numerical tolerance \( \varepsilon \) for inverting \( \mathbf{H} \) (Condition (14)), each application of the outer loop reduces the magnitude of the projection of \( \mathbf{w}^{(t)} \) onto \( \hat{\mathbf{u}}_l \) by a factor of \( \mathcal{O}(\delta \overline{\lambda}_1)^{-1} \eta \) \( \ll 1 \) given \( \eta \ll 1 \) (if we have a good initial estimator of \( \hat{\lambda}_1 \) and \( \delta \overline{\lambda}_1 = \Omega(1) \)).

Notice that if \( \mathbf{w}^{(t)} \) satisfies condition (13), our Equation (16) claims that \( \mathbf{w}^{(t+1)} = \mathbf{v}/\|\mathbf{v}\|_2 \)
satisfies Condition (13) as well. This condition is justified if \( \mathbf{w}(0) \) satisfies Condition (13), which is a conclusion from Equation (11).

Our second lemma characterizes the convergence rate of distributively solving the linear system \( \mathbf{Hw} = \mathbf{w}(t) \) in the outer loop of Algorithm 1. Recall that in Equation (2), \( \tilde{\mathbf{w}}^{(t+1)} = \mathbf{H}^{-1}\mathbf{w}(t) \) denote the exact solution of this linear system.

**Lemma 3.2.** Suppose the initial estimator \( \lambda_1 \) satisfies

\[
\lambda_1 - \hat{\lambda}_1 \geq \eta \geq \frac{1}{2} \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2. \tag{17}
\]

Then for each \( j = 0, 1, \ldots, (T' - 1) \), we have

\[
\| \mathbf{w}_{j+1}^{(t+1)} - \tilde{\mathbf{w}}^{(t+1)} \|_2 \leq \frac{2 \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2}{\eta} \| \mathbf{w}_j^{(t+1)} - \tilde{\mathbf{w}}^{(t+1)} \|_2. \tag{18}
\]

**Proof.** Deferred to Appendix A in the supplement. \( \square \)

Here \( \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2 \) on the RHS of (18) is due to the approximation using the Hessian matrix \( \mathbf{H}_1 \) on the first machine in place of original Hessian matrix \( \mathbf{H} \). As we will show later, by standard matrix concentration inequalities, we have \( \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2 = \mathcal{O}(\sqrt{d/m}) \) with high probability. As a consequence, the inner loop of Algorithm 1 has a contraction rate of order \( \mathcal{O}(\eta^{-1}\sqrt{d/m}) \), which is inversely proportional to the gap \( \lambda_1 - \hat{\lambda}_1 \) (due to the condition number of the Hessian \( \mathbf{H} \)).

Combining these two lemmas, we come to our first main theoretical result for the convergence rate of Algorithm 1.

**Theorem 3.3.** Let \( \kappa := \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2 = \mathcal{O}_P(\sqrt{d/m}) \). Assume

\[
2\eta \geq \lambda_1 - \hat{\lambda}_1 \geq \eta \geq \frac{1}{2} \kappa, \tag{19}
\]

and the initial eigenvector estimator \( \mathbf{w}(0) \) satisfies

\[
\sum_{t: \hat{\lambda}_t \leq (1-\delta) \hat{\lambda}_1} |\langle \hat{\mathbf{u}}_t, \mathbf{w}(0) \rangle|^2 \leq \frac{3}{4}.
\]
Then for each $T$ and $T'$ as the outer and inner iterations in Algorithm 1, respectively, and the relative eigenvalue gap $\delta \in (0, 1)$, we have

$$\sum_{t: \hat{\lambda}_t \leq (1-\delta) \hat{\lambda}_1} |\langle \hat{u}_t, \mathbf{w}(t) \rangle|^2 \leq \left( \frac{128\eta^2}{\delta^2 \hat{\lambda}_1^2} \right)^T + \frac{512 \eta}{1 - 128\eta^2/(\delta \hat{\lambda}_1)^2} \left( \frac{4\kappa^2}{\eta^2} \right)^{T'}.$$ (20)

Proof. Deferred to Appendix A in the supplement.

We can further simplify Equation (20) by choosing proper $\eta$ and $T'$.

**Corollary 3.4.** In particular, if $\eta \leq \delta \hat{\lambda}_1/16$, and we choose $T' = T$, and $\eta = (\kappa \delta \hat{\lambda}_1)^{1/2}/3 = \mathcal{O}_P(\sqrt{d/m})$, then the final output $\mathbf{w}(T)$ satisfies

$$\sum_{t: \hat{\lambda}_t \leq (1-\delta) \hat{\lambda}_1} |\langle \hat{u}_t, \mathbf{w}(T) \rangle|^2 \leq 257 \left( \frac{6\kappa}{\delta \hat{\lambda}_1} \right)^{2T}.$$ (21)

Proof. Combine additional conditions and Theorem 3.3.

As indicated in (21), when $6\kappa/\delta \hat{\lambda}_1 \ll 1$, our Algorithm 1 enjoys a linear convergence rate. Moreover, to ensure this convergence, when the absolute eigengap $\delta \hat{\lambda}_1$ is small, $\kappa = \mathcal{O}_P(\sqrt{d/m})$ needs to be smaller, i.e., $\kappa = o(\delta \hat{\lambda}_1)$ Recall that $\kappa := \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2$, which is defined in Theorem 3.3. This indicates that more samples are needed on each local machine. Finally, we provide a standard lemma to justify the claims that $\| \hat{\Sigma} - \hat{\Sigma}_1 \|_2 = \mathcal{O}_p \left( \sqrt{d/m} \right)$ and initial estimator conditions Equation (10) and Equation (11).

**Lemma 3.5.** If our samples $\mathbf{a}_i, i = 1, \ldots, n$ are sub-Gaussian($\sigma$) vectors, then with high probability, we have,

$$\| \hat{\Sigma} - \hat{\Sigma}_1 \|_2 = \mathcal{O} \left( \sqrt{\frac{d}{m}} \right).$$ (22)

The top eigenvalue on the first machine $\lambda_1(\mathbf{A}^\top \mathbf{A}/m)$ satisfies,

$$|\hat{\lambda}_1 - \lambda_1(\mathbf{A}^\top \mathbf{A}/m)| \leq \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2.$$ (23)
Furthermore, let \( w^{(0)} \) be the top eigenvector of \( \hat{\Sigma}_1 \) on the first machine. We have the following gap-free concentration bound for \( w^{(0)} \) and \( \hat{u}_1, \ldots, \hat{u}_d \),

\[
\sum_{l: \lambda_l \leq (1-\delta) \hat{\lambda}_1} \left| \langle \hat{u}_l, w^{(0)} \rangle \right|^2 \leq \frac{\| \hat{\Sigma} - \hat{\Sigma}_1 \|_2}{\delta \hat{\lambda}_1}.
\] (24)

Proof. Deferred to Appendix A in the supplement. \qed

3.2 Distributed top-\( L \)-dim principal subspace estimation

With the theoretical results for the top eigenvector estimation in place, we further present convergence analysis on the top-\( L \)-dim eigenspace estimation in Algorithm 2.

Let \( \tilde{U} = [\hat{u}_1, \ldots, \hat{u}_d] \) denote the column orthogonal matrix composed of all eigenvectors of \( \hat{\Sigma}_L \) whose associated eigenvalues have a relative gap \( \delta \) from the \( L \)-th largest eigenvalue \( \hat{\lambda}_L \), that is, \( \iota_\delta := \arg \min \{ l : \hat{\lambda}_l \leq (1-\delta) \hat{\lambda}_L \} \). We also use the notation \( \hat{\Sigma}^{(l)} = (I - V_{l-1}V_{l-1}^T) \hat{\Sigma}(I - V_{l-1}V_{l-1}^T) \) for \( l = 0, 1, \ldots, L - 1 \). Here \( V_l = [v_1, \ldots, v_l] \) consists of all the top-\( l \) eigenvector estimations and \( V_0 = 0 \). Notice that \( \hat{\Sigma}^{(l)} \) is just the matrix \( A^{(l)} A^{(l)}/n \) where \( A^{(l)} := [A_{1,l}, \ldots, A_{K,l}]^T \) and \( A_{k,l} \) is the projected data matrix on machine \( k \) \( (k = 1, \ldots, K) \) for the \( l \)-th eigenvector estimation.

We first provide our choices of initial eigenvalue estimates. For Algorithm 2 for the top-\( L \)-dim principal, let \( \hat{\Sigma}^{(l)}_k = A_{k,l}^T A_{k,l}/m \) and \( \hat{\Sigma}^{(l)} = K^{-1} \sum_{k=1}^K \hat{\Sigma}^{(l)}_k \) denote the local and global projected sample covariance matrices at the outer iteration \( l \). For the same constant \( \eta \) defined above in (9), we choose \( \bar{\lambda}_l = \lambda_1(\hat{\Sigma}_1^{(l)}) + 3\eta/2 \) for \( l = 1, \ldots, L \). This follows from

\[
\| \hat{\Sigma}^{(l)} - \hat{\Sigma}_1^{(l)} \|_2 = \left\| (I - V_l V_l^T)(\hat{\Sigma} - \hat{\Sigma}_1)(I - V_l V_l^T) \right\|_2 \leq \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2 \leq \frac{\eta}{2},
\]

which implies that,

\[ 2\eta \geq \bar{\lambda}_l - \lambda_1(\hat{\Sigma}^{(l)}) \geq \eta. \]
Our main result is summarized as follows.

**Theorem 3.6.** Let $\kappa = \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2 = O_P(\sqrt{d/m})$. Assume

$$2\eta \geq \lambda_l - \lambda_1(\hat{\Sigma}^{(l)}) \geq \eta \geq \frac{1}{2} \kappa,$$

for each $l = 1, 2, \ldots, L$, where $\lambda_1(\hat{\Sigma}^{(l)})$ denotes the largest eigen value of $\hat{\Sigma}^{(l)}$. Then we have

$$\| \tilde{U}^T V_L \|_2^2 \leq \frac{64\lambda_1 L^2}{\lambda L \delta} \sqrt{\left( \frac{128\eta^2}{\delta^2 \lambda L^2} \right)^T} + \frac{512 \eta}{1 - 128\eta^2/(\delta \lambda_L)^2} \left( \frac{4\kappa^2}{\eta^2} \right)^{T'}.$$  \hspace{1cm} (25)

**Proof.** Deferred to Appendix A in the supplement. \hfill \Box

By choosing specific settings of some parameters, the result in Theorem 3.6 can be simplified as shown in the following corollary.

**Corollary 3.7.** Similarly, if $\eta \leq \delta \lambda_1/16$, and we choose $T' = T$, and $\eta = (\kappa \delta \lambda_1)^{1/2}/3 = O_P(\sqrt{d/m})$, then our estimator $V_L$ satisfies

$$\| \tilde{U}^T V_L \|_2^2 = O \left( \frac{\lambda_1 L^2}{\lambda \delta \lambda_L} \left( \frac{6\kappa \lambda_1}{\delta \lambda_L} \right)^T \right).$$

**Remark 3.8.** It is worthwhile to note that we assume the data are evenly split only for the ease of discussions. In fact, the local sample size $m$ in our theoretical results is the sample size on the first machine (or any other machine that used to compute the estimation of Hessian $H$) in Algorithm 1 and Algorithm 2. As long as the sample size $m$ on the first machine is specified, our method does not depend on the partition of the entire dataset.

### 4 Applications

Our distributed PCA can be applied to a wide range of important applications. In this section, we discuss two applications to principal component regression and single index model. Model assumptions and theoretical results are provided in this section and further numerical experiments will be presented in Appendix D in the supplementary material.
4.1 Distributed PCA for principal component regression

Principal component regression (Jeffers, 1967; Jolliffe, 1982) is built on the following multivariate linear model,

\[ y = A\beta^* + \epsilon. \]  \hspace{1cm} (26)

In (26), \( A = [a_1, \ldots, a_n]^T \) is the \( n \times d \) observed covariate matrix with \( i.i.d. \) rows, where each \( a_i \) is a zero-mean random vector with the covariance matrix \( \Sigma \), \( \beta^* \) is the \( d \times 1 \) coefficient, and \( y \) is the \( n \times 1 \) response vector. The noise \( \epsilon = (\epsilon_1, \ldots, \epsilon_n)^T \) is the error term with \( \mathbb{E}(\epsilon_i) = 0 \) and \( \epsilon \) is independent from \( a \). Since our main purpose here is to illustrate PCR in our distributed algorithm, we assume that data dimension \( d \) is a constant. Of course, it would be interesting to extend to high-dimensional case, and we leave it for future investigation. Moreover, for the ease of technical derivation and presentation, we assume that \( \beta^* \) is normalized with \( \|\beta^*\|_2 = 1 \).

Our goal is to estimate the coefficient \( \beta^* \) from \( A, y \). Denote \( U_L = (u_1, \ldots, u_L), 1 \leq L \leq d \) the subspace spanned by the top-\( L \) eigenvectors of \( \Sigma \). In principal component regression (denoted as PCR below), \( \beta^* \) is assumed to lie in the same subspace, i.e.,

\[ \beta^* = U_L \gamma^*, \]

for some vector \( \gamma^* \in \mathbb{R}^L \). Our goal is to estimate \( \beta^* \).

Let \( \hat{\Sigma} = \frac{1}{n}A^TA \) be the sample covariance matrix with eigenvalues \( \hat{\lambda}_1 \geq \ldots \geq \hat{\lambda}_d > 0 \). Let \( \hat{U}_L = (\hat{u}_1, \ldots, \hat{u}_L) \) be the \( d \times L \) matrix associated with the first \( L \) eigenvectors of \( \hat{U} \), and we project our covariate data \( A \) on this estimated subspace, \( \tilde{A} = A\hat{U}_L \) and obtain an estimator \( \hat{\gamma} \) of \( \gamma^* \), which is the vector of estimated regression coefficients. This \( \hat{\gamma} \) is obtained by ordinary least squares regression of the response vector \( y \) on the projected data matrix.
Therefore, the standard PCR estimator is \( \hat{\beta} = \hat{U}_L \hat{\gamma} \).

In a single-machine setting, we can obtain \( \hat{U}_L \) directly from PCA on full empirical covariance matrix \( \hat{\Sigma} \). In a distributed environment, our data is splitted uniformly on \( K \) local machines. The data on each machine is denoted by \( A_k \in \mathbb{R}^{m \times d} \), \( y_k \in \mathbb{R}^{m \times 1} \) for \( k = 1, \ldots, K \). We therefore apply our Algorithm 2 to obtain a distributed version estimator of \( U_L \), denoted by \( V_L \). Now we have the corresponding projected data matrix \( \tilde{A}_k = A_k V_L \) on each machine. The \( \tilde{A}_k^\top \tilde{A}_k \), \( \tilde{A}_k^\top y_k \) are then computed locally and collected by the central machine. Then the central machine computes an OLS estimator based on \( y \) and \( \tilde{A} \),

\[
\tilde{\gamma} = \left( \sum_{k=1}^{K} \tilde{A}_k^\top \tilde{A}_k \right)^{-1} \left( \sum_{k=1}^{K} \tilde{A}_k^\top y_k \right) = \left( \tilde{A}^\top \tilde{A} \right)^{-1} \tilde{A}^\top y. \tag{27}
\]

Finally, our distributed estimator is obtained from \( \tilde{\beta} = V_L \tilde{\gamma} \).

We first make some standard assumptions on general PCR model.

**Assumption 4.1.** Under the PCR model, we further assume that

(1) \( \lambda_L - \lambda_{L+1} > 0 \);

(2) Noise term \( \{\epsilon_i\}_{i=1}^n \) are independent sub-Gaussian(\( \sigma_1^2 \)) random variables and covariate \( \{a_i\}_{i=1}^n \) are independent sub-Gaussian(\( \sigma_2^2 \)) vectors.

Note that for the PCR application, the item (1) is necessary to guarantee the identifiability of the column space \( U_L = \{u_1, \ldots, u_L\} \), i.e., the top-\( L \) eigenspace of population covariance matrix \( \Sigma \). Furthermore, by standard matrix concentration, we have, with high probability, that \( \hat{\lambda}_L > \hat{\lambda}_{L+1} \). Thus, when we apply our distributed estimation using Algorithm 2, we explicitly set the relative eigengap threshold to be \( \delta = (\hat{\lambda}_L - \hat{\lambda}_{L+1})/\hat{\lambda}_L \).
Proposition 4.2 below first describes the upper bound of estimation error for the usual PCR result where data matrix is on one machine.

**Proposition 4.2.** Under Assumption 4.1, the standard single-machine estimator $\hat{\beta}$ has,

$$
\| \hat{\beta} - \beta^* \|_2 \leq \sqrt{2} C_0 \lambda_1^{-1} \sigma_1 \sqrt{\frac{d}{n}} + 2^{5/2} \sigma_2 \sqrt{\frac{d}{n}} \frac{\sqrt{L}}{\lambda_L - \lambda_{L+1}},
$$

(28)

where $C_0 > 0$ is a constant.

**Proof.** This result is standard and we include the proof in Appendix B in the supplement for the purpose of completeness.

We would like to make some remarks on Proposition 4.2. By Theorem 5.39 in Vershynin (2012), with high probability $\hat{\lambda}_L \geq \lambda_L + o(1)$. Therefore, $\hat{\lambda}_L^{-1}$ is bounded with high probability, i.e., $\hat{\lambda}_L^{-1} \leq \text{constant} + o_p(1)$. This indicates that the oracle estimator of PCR enjoys a statistical convergence rate of order $O_p(\sqrt{d/n})$, which is of the same order as $\| \Sigma - \hat{\Sigma} \|_2$.

Now we are ready to discuss the case of distributed PCR. We define the following matrix, $G$, to quantify the estimation error between some estimator $V_L$ and the eigenspace estimator $\hat{U}_L$ on the full data covariance $\hat{\Sigma}$ using the standard PCA,

$$
G = V_L^T \hat{U}_{-L},
$$

(29)

where $\hat{U}_{-L} = [\hat{u}_{L+1}, \ldots, \hat{u}_d]$. Furthermore, we let $g = \| G \|_2$, which is used as error measurement in Theorem 3.6 if we set eigengap threshold $\delta$ to be $(\hat{\lambda}_L - \hat{\lambda}_{L+1})/\hat{\lambda}_L$. With these notions in hand, we introduce the following theorem on distributed estimator $\tilde{\beta}$.

**Theorem 4.3.** Under Assumption 4.1, with high probability, our distributed estimator $\tilde{\beta}$ satisfies,

$$
\| \tilde{\beta} - \beta^* \|_2 \leq \sqrt{2} C_0 \sigma_1 \mu^{-1} \sqrt{\frac{d}{n}} + 2^{3/2} \sigma_2 \left(2 + \mu^{-1} \nu\right) \left(\sqrt{\frac{d}{n}} \frac{\sqrt{L}}{\lambda_L - \lambda_{L+1}} + \sqrt{2g}\right),
$$

(30)

where $C_0 > 0$ is a constant. Here $\mu = \hat{\lambda}_L - 4g \hat{\lambda}_1$ and $\nu = 4g \hat{\lambda}_1$. 

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Proof. Deferred to Appendix B in the supplement.

Notice that when $V_L$ is $\hat{U}$ (up to an orthogonal transformation), we have $g = \nu = 0$, and $\mu = \hat{\lambda}_L$. Then the bound (30) in Theorem 4.3 is the same as the bound (28) in Proposition 4.2. When our estimator $V_L$ has a positive estimation error, if we estimate $\hat{U}_L$ using Algorithm 2, then with Theorem 3.6, we have $g = \|G\|_2 \leq \varepsilon_L$ where

$$
\varepsilon_L^2 = \frac{64\hat{\lambda}_1 L^2}{\hat{\lambda}_L \delta} \sqrt{\left( \frac{128\eta^2}{\delta^2 \hat{\lambda}_L^2} \right)^T + \frac{512\eta}{1 - 128\eta^2} \left( \frac{4\kappa^2}{\eta^2} \right)^T}.
$$

Here we take $\delta$ to be the relative eigengap, i.e., $\delta = (\hat{\lambda}_L - \hat{\lambda}_{L+1})/\hat{\lambda}_L$. Furthermore, if the estimation error $g \leq \varepsilon_L = o(1)$, we have $\mu = \hat{\lambda}_L - 4g\hat{\lambda}_1 > 0$ and Equation (30) can be simplified as,

$$
\|\tilde{\beta} - \beta^*\|_2 = \mathcal{O}\left( \sqrt{\frac{d}{n}} \right) + o(1), \tag{31}
$$

which is the optimal parametric estimation rate.

4.2 Distributed PCA for single index model

In a standard single index model (denoted as SIM below), we assume,

$$
y = f(\langle \beta^*, a \rangle) + \epsilon,
$$

where $y \in \mathbb{R}$ is the response, $a$ is the $d$-dimensional covariate vector, $\beta^* \in \mathbb{R}^d$ is the parametric component and $\epsilon$ is a zero-mean noise that is independent of $a$. Here, the so-called link function $f : \mathbb{R} \mapsto \mathbb{R}$ is the nonparametric component. We also focus on the low-dimensional setting where $d$ does not grow with the sample size $n$. For the model identifiability, we assume that $\|\beta^*\|_2 = 1$ since $\|\beta^*\|_2$ can be absorbed into $f$. Following Li (1992); Janzamin et al. (2014) and references therein, we can use the second order Stein’s identity to estimate $\beta^*$. 

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**Proposition 4.4.** Assume that the density \( p \) of \( \mathbf{a} \) is twice differentiable. In addition, we define the second-order score function \( T : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d} \) as

\[
T(\mathbf{a}) = \nabla^2 p(\mathbf{a})/p(\mathbf{a}).
\]

Then, for any twice differentiable function \( g : \mathbb{R}^d \rightarrow \mathbb{R} \) such that \( \mathbb{E}[\nabla^2 g(\mathbf{a})] \) exists, we have

\[
\mathbb{E}[g(\mathbf{a}) \cdot T(\mathbf{a})] = \mathbb{E} [\nabla^2 g(\mathbf{a})].
\]

**Proof.** Please refer to Theorem 6 in Janzamin et al. (2014) and set \( m = 2 \).

Now we consider the SIM with Gaussian distribution as a special case, where \( \mathbf{a} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_d) \). The second order score function now becomes

\[
T(\mathbf{a}) = \mathbf{a}\mathbf{a}^\top - \mathbf{I}_d.
\]

By Proposition 4.4 we have

\[
\mathbb{E}[y (\mathbf{a}\mathbf{a}^\top - \mathbf{I}_d)] = C_0 \cdot \beta^* \beta^{*\top},
\]

(32)

where \( C_0 = 2 \mathbb{E} [f'' (\langle \mathbf{a}, \beta^* \rangle)] \).

Therefore, one way to estimator \( \beta^* \) is to obtain the leading eigenvector of \( \mathbb{E}[y (\mathbf{a}\mathbf{a}^\top - \mathbf{I}_d)] \) from samples. Given \( n \) i.i.d. sample \( \{\mathbf{a}_i, y_i\}_{i=1}^n \), we can calculate the estimator \( \hat{\beta} \) by extracting the leading eigenvector of \( \frac{1}{n} \sum_{i=1}^n y_i \cdot (\mathbf{a}_i \mathbf{a}_i^\top - \mathbf{I}_d) \), the empirical estimation of \( \mathbb{E}[y (\mathbf{a}\mathbf{a}^\top - \mathbf{I}_d)] \). This can also be extended to our distributed setting, where we estimate \( \hat{\beta} \) by \( \tilde{\beta} \) from the distributed PCA Algorithm 1.

Let \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d \) denote the eigenvalues of population matrix \( \mathbb{E}[y (\mathbf{a}\mathbf{a}^\top - \mathbf{I}_d)] \) and \( \hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \ldots \geq \hat{\lambda}_d \) the eigenvalues for the empirical matrix \( \frac{1}{n} \sum_{i=1}^n y_i \cdot (\mathbf{a}_i \mathbf{a}_i^\top - \mathbf{I}_d) \) calculated with pooled data. Before presenting our theoretical results, we make some standard assumptions.
**Assumption 4.5.** Under the Gaussian SIM model given above, we further assume that

1. We assume $f$ and $a$ are such that $E[f''(\langle a, \beta^* \rangle)] > 0$, and moreover, $f(\langle \beta^*, a \rangle)$ is bounded.

2. We assume the noise term $\{\epsilon_i\}_{i=1}^n$ to be independent, zero-mean sub-Gaussian($\sigma$) random variables.

Item (1) is commonly assumed in many references, for example, Definition 2.6 in Yang et al. (2017). We further make a boundedness assumption on $f(\cdot)$. This assumption make use of the fact that $a$ is spherical Gaussian, thus with high probability, $\langle \beta^*, a \rangle$ is bounded and $f(\cdot)$ only need to be finite in this domain.

Still, we consider the single-machine case first. The following proposition quantifies the statistical rate of convergence of the non-distributed estimator $\hat{\beta}$.

**Theorem 4.6.** Under Gaussian SIM model and Assumption 4.5, our estimator $\hat{\beta}$ satisfies

$$
\min_{t \in \{-1, +1\}} \|t\hat{\beta} - \beta^*\|_2 = \tilde{O}_p \left( \frac{d}{\sqrt{n}} \right),
$$

(33)

with high probability.

**Proof.** The proof is provided in Appendix C in the supplement. \qed

We can extend the Gaussian SIM model to our distributed framework where data are stored on different machines. The transformed “covariance matrix” on each machine $k$ has the form $\frac{1}{m} \sum_{j=1}^m y_j^{(k)}(a_j^{(k)}a_j^{(k)\top} - I_d)$ for $k = 1, \ldots, K$. Then it is straightforward to apply Algorithm 1 to obtain a distributed estimation $\tilde{\beta}$ of $\beta^*$. Combining the results in Theorem 3.3, Corollary 3.4, and Theorem 4.6, we can obtain the non-asymptotic upper bound for our distributed estimator $\tilde{\beta}$. 
Proposition 4.7. In a distributed environment, if we estimate $\beta^*$ with $\tilde{\beta}$ using Algorithm 1. We set the numbers of inner iterations and outer iterations to be $T$ simultaneously. Under Assumption 4.5 and if $\eta \leq \delta \hat{\lambda}_1/16$ in Corollary 3.4, our distributed estimator $\tilde{\beta}$ satisfies,

$$\min_{t \in \{-1, +1\}} \|t\tilde{\beta} - \beta^*\|_2 \leq \tilde{O}_p \left( \frac{d}{\sqrt{n}} \right) + O_p \left( \left[ \frac{d \log d}{m} \right]^{T/2} \right).$$  \tag{34}

Proposition 4.7 indicates that when the number of iterations $T$ is sufficiently large, the first error term in (34) will dominate the second one and therefore our estimator $\tilde{\beta}$ will have the convergence rate of $\tilde{O}_p (d / \sqrt{n})$.

5 Numerical Study

In this section, we provide simulation experiments to illustrate the empirical performance of our distributed PCA algorithm.

Our data follows a normal distribution, $E[a] = 0$ and the population covariance matrix $E[aa^\top] = \Sigma$ is generated as follows:

$$\Sigma = U \Lambda U^T,$$

where $U$ is an orthogonal matrix generated randomly and $\Lambda$ is a diagonal matrix. Since our experiments mainly estimate the top-3 eigenvectors, $\Lambda$ has the following form,

$$\Lambda = \text{diag} (1 + 3\delta, 1 + 2\delta, 1 + \delta, 1, \ldots, 1).$$  \tag{35}

For example, when the relative eigengap $\delta$ is 1, $\Lambda = \text{diag}(4, 3, 2, 1, \ldots, 1)$.

For orthogonal matrix $U = [u_{ij}] \in \mathbb{R}^{d \times d}$, we first generate all elements $u_{ij}, i, j = 1, \ldots, d$ such that they are $i.i.d.$ standard normal variables. We then use Gram-Schmidt process to orthonormalize the matrix and obtain the $U$.

We will compare our estimator with the following two estimators:
(1) Oracle estimator: the PCA estimator is computed in the single-machine setting with pooled data, i.e., we gather all the sampled data and compute the top eigenspace of \( \hat{\Sigma} = \frac{1}{n} A A^\top \), where \( A \in \mathbb{R}^{n \times d} \) is the data matrix.

(2) DC estimator (Algorithm 1 in Fan et al. (2019)): it first computes the top-\( L \)-dim eigenspace estimation \( \hat{U}_L^{(k)}, k = 1, \ldots, K \) on each machine, and merges every local result together with \( \tilde{\Sigma} = \frac{1}{K} \sum_{k=1}^{K} \hat{U}_L^{(k)} \hat{U}_L^{(k)^\top} \). The final estimator is given by the eigenvalue decomposition of \( \tilde{\Sigma} \).

Note that all the reported estimation errors are computed based on the average of 100 Monte-Carlo simulations. Since the standard deviations of Monte-Carlo estimators for all the methods are similar and sufficiently small, we omit standard deviation terms in the following Figures and only report the average errors for better visualization. As shown in the following subsections, our distributed algorithm gets to a very close performance with the oracle one when the number of outer iterations \( T \) is large enough and outperforms its divide-and-conquer counterpart.

For distributed PCA, we adopt the following error measurements from the bound (20) and bound (25) with population eigenvectors replacing the oracle estimator. To be more specific, for top eigenvector case, with the estimator \( \hat{u}_1 \), population eigenvectors \( u_1, \ldots, u_d \), population eigenvalues \( \lambda_1, \ldots, \lambda_d \) and relative eigenvalue gap \( \delta \in (0, 1) \), the error measurement is defined as

\[
\text{error}(\hat{u}_1) = \sum_{l:\lambda_l \leq (1-\delta)\lambda_1} |\langle u_l, \hat{u}_1 \rangle|^2.
\]

(36)

As for the top-\( L \)-dim eigenspace estimation, let \( \tilde{U} = [u_{l_\delta}, \ldots, u_d] \) be the column orthogonal matrix composed of all eigenvectors of population covariance \( \Sigma \) whose associated eigenvalues have a relative gap \( \delta \) from the \( L \)-th largest eigenvalue \( \lambda_L \). That is, \( l_\delta := \arg\min \{l : \).
Recall that $\hat{U}_L$ is the estimator the top-$L$ eigenvectors. Then the corresponding error should be

$$\text{error}(\hat{U}_L) = \left\| \tilde{U}^\top \hat{U}_L \right\|_2^2.$$  \hfill (37)

### 5.1 Varying the number of outer iterations

In this section, we present tests on how the performance of our distributed PCA changes with the number of outer iterations $T$ in Algorithm 1. Consider data dimension $d$ to be 50, sample size on each machine to be 500, and the number of machines to be 200, i.e., $a \in \mathbb{R}^{50}$,
Figure 2: Comparison between algorithms when the number of outer iterations varies, under the same setting as in Figure 1. Subfigures (a) to (c) represent the experiments with 5 inner loops. Subfigures (d) to (f) represent the experiments with 10 inner loops. Eigengap $\delta$ is fixed to be 2.0.

We will report the logarithmic error. As shown in Theorem 4.6, the logarithmic error follows an approximately linear decrease with respect to the number of outer iterations. A linear relationship between the number of outer iterations and logarithmic error verifies our theoretical findings.

We now check the performance of these three approaches (oracle one, our method and DC method) under the setting of a small eigen-gap. Specifically, we let eigengap $\delta$ to be 1.0 and 2.0. Our data is drawn independently, and $\mathbf{a}_i \sim \mathcal{N}(0, \Sigma)$ for $i = 1, \ldots, mK$. We vary the number of outer iterations $T$ to evaluate the performance.
Figure 3: Comparison between algorithms when eigen-gap varies. The x-axis is the reciprocal of eigengap and the y-axis is the logarithmic error.

As we fix the total sample size $n = 10^5$, the errors of oracle estimator and DC estimator should be constants (illustrated by two horizontal dash lines in the graphs since they are not iterative algorithms). As shown below in Figure 1 and Figure 2, our method converges to the oracle estimator in around 20 iterations and outperforms the DC method. Moreover, as expected, we observe a approximately linear relation between logarithmic error and the number of outer iterations. We also observe that, empirically, setting the number of inner iterations $T' = 5$ in Algorithm 1 is good enough for most cases.

5.2 Varying the eigengap

In the convergence analysis of both our distributed algorithm and DC method, eigengap plays a central role in the error bound. When the eigengap between $\lambda_L$ and $\lambda_{L+1}$ becomes smaller, the estimation task turns to be harder and more rounds are needed for the same error. Theorem 4 in Fan et al. (2019) also shows a similar conclusion. In this part, we continue our experiment in Section 5.1, and examine the relationship between estimation error and eigengap.

We fix the number of inner iterations to be 10, and the number of outer iterations to be
40, which, from Section 5.1, is large enough for top-3-dim eigenspace. We still consider data dimension \( d \) to be 50, sample size on each machine to be 500, and the number of machines to be 200, i.e., \( \mathbf{a} \in \mathbb{R}^{50}, m = 500 \) and \( K = 200 \). Under this setting, we vary \( \delta \) in (35) and the results is shown in Figure 3. In Figure 3, the logarithmic error increases with respect to \( 1/\delta \), which agrees with our theoretical findings. Furthermore, our estimator has the same performance as the oracle one.

### 5.3 Varying the number of machines for asymmetric innovation distributions

In this section, we compare our method to the DC method by varying the number of local machines. As mentioned in Theorem 4 in Fan et al. (2019), DC method has a slower convergence rate (of order \( O(\rho \sqrt{Lr/n}) + O(\rho^2 \sqrt{Lr/m}) \) instead of the optimal rate \( O(\rho \sqrt{Lr/n}) \)) when the number of machines is greater than \( O(m/(\rho^2 r)) \) in the asymmetric innovation distributions (defined in Section 1.1) setting. Here \( \rho \) is the condition number of the population covariance matrix, i.e., \( \rho = \lambda_1/(\lambda_L - \lambda_{L+1}) \), and \( r = \text{Tr}(\Sigma)/\lambda_1 \) is the effective rank of \( \Sigma \).

We set data dimension \( d \) to be 50, local sample size to be 500, i.e., \( \mathbf{a} \in \mathbb{R}^{50}, m = 500 \). We choose eigengap \( \delta \) to be 0.5, thus \( \Lambda = \text{diag}(2.5, 2, 1.5, 1, \ldots, 1) \). Here, without sticking on our Gaussian setting, we consider to use skew-distributed random variables. In particular, we generate \( \mathbf{a} = [a_1, \ldots, a_d]^{\top} \in \mathbb{R}^d \) from beta distribution family such that for each \( a_i, i = 1, \ldots, d \), we set its mean to be zero, variance to be \( \Lambda_{ii} \) and skewness to be 4 or 6, respectively.

We set the iteration parameters as in Section 5.2 and the number of machines is varied from 100 to 51, 200. Our results are shown in Figure 4. As can be seen from Figure 4, our method achieves the same statistical convergence rate as the oracle one. When the number of machines is small, the estimation error of the DC method also decreases at the same rate as
Figure 4: Comparison between algorithms when the number of machines varies. The $x$-axis is the log the number of machines and the $y$-axis is the logarithmic error. Subfigures (a) to (c) represent the experiments of top-1-dim to top-3-dim eigenvector estimation with skewness 4.0 and (d) to (f), 6.0.

the number of machines increases. However, the estimation error the of DC method becomes flat (or decreases at a much slower rate) when the number of machines is larger than a certain threshold. In that regime, our approach is still comparable to its oracle counterpart.

We also conduct simulation studies on principal component regression and Gaussian single index model cases and compare our approach with the oracle and the DC ones. Due to the space limitation, we defer these results to Appendix D in the supplementary material.
6 Discussions and Future Work

In this paper, we address the problem of distributed estimation for principal eigenspace. Our proposed multi-round method achieves fast convergence rate. Furthermore, we establish an eigenvalue gap-free error bound for our method, which is superior to traditional error bound. The insight behind our work is the combination of shift-and-invert preconditioning and convex optimization, with the adaption into distributed environment. This distributed PCA algorithm refines the divide-and-conquer scheme and removes the constraint on the number of machines from previous methods.

One important future direction is to further investigate the principal eigenspace problem under distributed settings. Specifically, computational approaches and theoretical tools can be established for other types of PCA problems, such as PCA in high dimension (see, e.g., Johnstone et al. (2001); Fan and Wang (2017); Cai et al. (2018)) and sparse PCA (see, e.g., Johnstone and Lu (2009); Cai et al. (2013); Vu et al. (2013)).

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Appendix A  Proofs of Distributed PCA

Proof of Lemma 3.1

Proof. Write \( v = H^{-1}w + e \), where \( \|e\|_2 \leq \varepsilon \). Since \( H^{-1} = (\lambda_1 I - \hat{\Sigma})^{-1} = \sum_{l=1}^{d}(\lambda_1 - \hat{\lambda}_l)^{-1}\hat{u}_l\hat{u}_l^\top \), we have, for each \( l = 1, \ldots, d \),

\[
\langle \hat{u}_l, v \rangle = (\lambda_1 - \hat{\lambda}_l)^{-1}\langle \hat{u}_l, w \rangle + \langle \hat{u}_l, e \rangle.
\]  

(38)

This can yield a lower bound on \( \|v\|_2 \),

\[
\|v\|_2^2 = \sum_{l=1}^{d} \|\langle \hat{u}_l, v \rangle\|^2 \geq \sum_{l:\hat{\lambda}_l > (1-\delta)\hat{\lambda}_i} \left[ \frac{1}{2}(\lambda_1 - \hat{\lambda}_l)^{-2} \|\langle \hat{u}_l, w \rangle\|^2 - \|\langle \hat{u}_l, e \rangle\|^2 \right]
\]

\[
\geq (32\eta^2)^{-1} - \|e\|_2^2 \geq (32\eta^2)^{-1} - \varepsilon^2 \geq (64\eta^2)^{-1},
\]

(39)

where we used the upper bound of \( \lambda_1 - \hat{\lambda}_l \), and the conditions (13) and (14) in Lemma 3.1.

On the other hand, for each \( l \) such that \( \hat{\lambda}_l \leq (1-\delta)\hat{\lambda}_i \), we have \( \lambda_1 - \hat{\lambda}_l \geq \hat{\lambda}_1 - \hat{\lambda}_l \geq \delta \hat{\lambda}_1 \).

Consequently, equation (38) implies

\[
|\langle \hat{u}_l, v \rangle| \leq (\delta \hat{\lambda}_1)^{-1} |\langle \hat{u}_l, w \rangle| + |\langle \hat{u}_l, e \rangle| \leq (\delta \hat{\lambda}_1)^{-1} |\langle \hat{u}_l, w \rangle| + \varepsilon.
\]

A combination of the last two displays yields the first claimed bound. Similarly, the second claim bound follows by combining inequality (39) with

\[
\sum_{l:\hat{\lambda}_l \leq (1-\delta)\hat{\lambda}_i} |\langle \hat{u}_l, v \rangle|^2 \leq 2(\delta \hat{\lambda}_1)^{-2} \sum_{l:\hat{\lambda}_l \leq (1-\delta)\hat{\lambda}_i} |\langle \hat{u}_l, w \rangle|^2 + 2 \sum_{l:\hat{\lambda}_l \leq (1-\delta)\hat{\lambda}_i} |\langle \hat{u}_l, e \rangle|^2
\]

\[
\leq 2(\delta \hat{\lambda}_1)^{-2} \sum_{l:\hat{\lambda}_l \leq (1-\delta)\hat{\lambda}_i} |\langle \hat{u}_l, w \rangle|^2 + 2\varepsilon^2.
\]

\[\square\]
Proof of Lemma 3.2

Proof. It is easy to verify the following two identities:

\[ \tilde{w}^{(t+1)} = w_j^{(t+1)} - H^{-1}(Hw_j^{(t+1)} - w^{(t)}), \]
\[ w_{j+1}^{(t+1)} = w_j^{(t+1)} - H_1^{-1}(Hw_j^{(t+1)} - w^{(t)}). \]

By taking the difference we obtain

\[ \|w_{j+1}^{(t+1)} - \tilde{w}^{(t+1)}\|_2 = \|(H^{-1} - H_1^{-1})(Hw_j^{(t+1)} - w^{(t)})\|_2 \]
\[ = \|(I - H_1^{-1}H)(w_j^{(t+1)} - H^{-1}w^{(t)})\|_2 \]
\[ \leq \|I - H_1^{-1}H\|_2 \|w_j^{(t+1)} - \tilde{w}^{(t+1)}\|_2. \]

We bound the first factor on the r.h.s. as

\[ \|I - H_1^{-1}H\|_2 \leq \|H_1^{-1}\|_2 \|H_1 - H\|_2 \leq \frac{2}{\eta} \|\hat{\Sigma} - \hat{\Sigma}_1\|_2, \]

where the last step follows from the fact \( H_1 - H = -(\hat{\Sigma} - \hat{\Sigma}_1) \), and the inequality

\[ \|H_1^{-1}\|^{-1}_2 = \lambda_{\min}(H_1) = \lambda_{\min}(\lambda_1 I - \hat{\Sigma} + (\hat{\Sigma} - \hat{\Sigma}_1)) \geq \lambda_{\min}(\lambda_1 I - \hat{\Sigma}) - \|\hat{\Sigma} - \hat{\Sigma}_1\|_2 \]
\[ \geq \eta - \|\hat{\Sigma} - \hat{\Sigma}_1\|_2 \geq \eta/2, \]

where \( \lambda_{\min}(A) \) denotes the smallest singular value of symmetric matrix \( A \).

\[ \square \]

Proof of Theorem 3.3

Proof. Applying Lemma 3.2, we have (recall \( w_0^{t+1} = w^{t}_T \))

\[ \|w_T^{t+1} - H^{-1}w_T^t\|_2 \leq \left( \frac{2\kappa}{\eta} \right)^T \|w_T^t - H^{-1}w_T^t\|_2 \leq \left( \frac{2\kappa}{\eta} \right)^T \frac{2}{\eta} \epsilon_T^r, \]

39
where we used the fact that \( \| I - H^{-1} \|_2 \leq 1 + \| H^{-1} \|_2 = 1 + (\lambda_1 - \hat{\lambda}_1)^{-1} \leq 2/\eta \), and \( \| w_T \|_2 = 1 \). Now we can recursively apply inequality (16) with \( \varepsilon \leftarrow \varepsilon_T \) to obtain

\[
\sum_{t: \lambda_t \leq (1-\delta) \hat{\lambda}_1} |\langle \hat{\mathbf{u}}_t, \mathbf{w}^{(t)} \rangle|^2 \leq \frac{128\eta^2}{\delta^2 \lambda_1^2} \sum_{t: \lambda_t \leq (1-\delta) \hat{\lambda}_1} |\langle \hat{\mathbf{u}}_t, \mathbf{w}^{(t-1)} \rangle|^2 + 128\eta^2 \varepsilon_T^2 
\]

\[
\leq \left( \frac{128\eta^2}{\delta^2 \lambda_1^2} \right)^2 \sum_{t: \lambda_t \leq (1-\delta) \hat{\lambda}_1} |\langle \hat{\mathbf{u}}_t, \mathbf{w}^{(t-2)} \rangle|^2 + \left( 1 + \frac{128\eta^2}{\delta^2 \lambda_1^2} \right) 128\eta^2 \varepsilon_T^2 
\]

\[
\leq \ldots \leq \left( \frac{128\eta^2}{\delta^2 \lambda_1^2} \right)^T \sum_{t: \lambda_t \leq (1-\delta) \hat{\lambda}_1} |\langle \hat{\mathbf{u}}_t, \mathbf{w}^{(0)} \rangle|^2 + 128\eta^2 \varepsilon_T^2, \sum_{t=0}^T \left( \frac{128\eta^2}{\delta^2 \lambda_1^2} \right)^t
\]

\[
\leq \left( \frac{128\eta^2}{\delta^2 \lambda_1^2} \right)^T + \frac{128\eta^2 \varepsilon_T^2}{1 - 128\eta^2 / (\delta \hat{\lambda}_1)^2}.
\]

\[ \square \]

**Proof of Lemma 3.5**

*Proof.* By Corollary 5.50 in Vershynin (2012), with probability at least \( 1 - 2e^{-d\sigma^2/C} \),

\[
\| \hat{\Sigma} - \Sigma \|_2 \leq \| \hat{\Sigma} - \Sigma \|_F \leq \sqrt{\frac{d}{n} \sigma},
\]

and

\[
\| \hat{\Sigma}_1 - \Sigma \|_2 \leq \| \hat{\Sigma}_1 - \Sigma \|_F \leq \sqrt{\frac{d}{m} \sigma},
\]

where \( C \) is a constant which only depends on the sub-Gaussian norm of the random vector \( \mathbf{a} \). Therefore, our first inequality (22) is a direct result of above matrix concentrations as well as triangle inequality for matrix spectral norm.

Denote \( \hat{\mathbf{u}}_1 \) and \( \mathbf{w}^{(0)} \) to be the top eigenvector for \( \hat{\Sigma} \) and \( \hat{\Sigma}_1 \), without loss of generality, we can assume \( \hat{\lambda}_1 > \lambda_1(A_1^\top A_1/m) \), then we have

\[
|\hat{\lambda}_1 - \lambda_1(A_1^\top A_1/m)| = \hat{\mathbf{u}}_1^\top \hat{\Sigma} \hat{\mathbf{u}}_1 - \mathbf{w}^{(0)}^\top \hat{\Sigma}_1 \mathbf{w}^{(0)}
\]

\[
\leq \hat{\mathbf{u}}_1^\top \hat{\Sigma} \hat{\mathbf{u}}_1 - \hat{\mathbf{u}}_1^\top \hat{\Sigma}_1 \hat{\mathbf{u}}_1
\]

\[
\leq \| \hat{\Sigma} - \hat{\Sigma}_1 \|_2.
\]
With Davis-Kahan Theorem (Yu et al., 2014), it is easy to see,
\[
\sum_{l : \tilde{\lambda}_l \leq (1 - \delta) \hat{\lambda}_1} \left| \langle \tilde{u}_l, \hat{w}^{(0)} \rangle \right|^2 \leq \frac{\| \hat{\Sigma} - \hat{\Sigma}_1 \|_2}{\delta \hat{\lambda}_1}.
\]

Proof of Theorem 3.6

Proof. Our proof adapts the proof of Theorem 4.1(a) in Allen-Zhu and Li (2016) to our settings.

Let \( \hat{\mu} = \left\| \hat{\Sigma}^{(L-1)} \right\|_2 \). Due to the Courant minimax principle, we have \( \mu \geq \hat{\lambda}_L \).

Note that column vectors in \( V_l \) are already eigenvectors of \( \hat{\Sigma}^{(l)} \) with eigenvalues zero. Let \( W_l \) be column orthogonal matrix whose columns are eigenvectors in \( V^\perp_l \) of \( \hat{\Sigma}^{(l)} \) with eigenvalues in the range \( [0, (1 - \delta + \tau_l) \hat{\mu}] \), where \( \tau_l = \frac{l}{2L} \delta \), for \( l = 0, 1, \ldots, L \).

We will show that for each \( l = 0, 1, \ldots, L \), there exists a matrix \( Q_l \) such that
\[
\left\| \tilde{U} - W_l Q_l \right\|_2 \leq \varepsilon_l \in [0, 1) \quad \text{and} \quad \| Q_l \|_2 \leq 1,
\] (40)
for some sequence \( \{ \varepsilon_l \}_{l=1}^L \) of small numbers. This would imply our claimed bound. In fact, the first inequality in the preceding display implies \( \left\| I - \tilde{U}^\top W_l Q_l \right\|_2 \leq \varepsilon_l \). Therefore, the smallest singular value of \( \tilde{U}^\top W_l Q_l \) is at least \( 1 - \varepsilon_l > 0 \). This lower bound combined with \( \| Q_l \|_2 \leq 1 \) implies the smallest singular value of \( \tilde{U}^\top W_L \) to be at least \( 1 - \varepsilon_L \), or
\[
I - \tilde{U}^\top W_L W_L^\top \tilde{U} \preceq 1 - (1 - \varepsilon_L)^2 I.
\]

Now since \( V_L \) is (column) orthogonal to \( W_L \), we obtain
\[
\tilde{U}^\top V_l V_l^\top \tilde{U} \preceq \tilde{U}^\top (I - W_L W_L^\top) \tilde{U} \preceq 2 \varepsilon_L I,
\]
which implies \( \left\| \tilde{U}^\top V_L \right\|_2 \leq \sqrt{2 \varepsilon_L} \).

When \( l = 0 \), we simply choose \( W_0 = \tilde{U} \), \( \varepsilon_0 = 0 \) and \( Q_0 = I \). Suppose for every \( l \in \{0, \ldots, L - 1\} \), there exists a matrix \( Q_l \) with \( \| Q_l \|_2 \leq 1 \) satisfying \( \left\| \tilde{U} - W_l Q_l \right\|_2 \leq \varepsilon_l \) for some \( \varepsilon_l \in [0, 1) \). Now we construct \( Q_{l+1} \) as follows.
Since \( \kappa = \left\| \hat{\Sigma} - \bar{\Sigma}_1 \right\|_2 \geq \left\| (I - V_l V_l^\top)(\hat{\Sigma} - \bar{\Sigma}_1)(I - V_l V_l^\top) \right\|_2 \), we can apply Theorem 3.3 to \( w_{l+1} \) with \( \delta \leftarrow \delta/2 \) to obtain (note that columns of \( W_l \) and \( V_l \) correspond to eigenvectors of \( \hat{\Sigma}^{(l)} \) with eigenvectors less than or equal to \( (1 - \delta + \tau_l) \left\| \hat{\Sigma}^{(L-1)} \right\|_2 \leq (1 - \delta/2) \left\| \hat{\Sigma}^{(l)} \right\|_2 \))

\[
\left\| W_l^\top w_{l+1} \right\|_2^2 \leq \epsilon_{T,T}^{(l)} \quad \text{and} \quad \left\| V_l^\top w_{l+1} \right\|_2^2 \leq \epsilon_{T,T}^{(l)},
\]

where \( \epsilon_{T,T}^{(l)} = \left( \frac{1}{\delta^2 \lambda_1(\hat{\Sigma}^{(l)}_T)^2} \right) + \frac{512 \eta}{1 - 128 \eta^2/(\delta \lambda_1(\hat{\Sigma}^{(l)}_T)^2)} \left( \frac{4 \kappa^2}{\eta^2} \right)^T \leq 1/2 \). Since \( w_{l+1} \) is the projection of \( w_{l+1} \) into \( V_l^\perp \), we have

\[
\left\| W_l^\top v_{l+1} \right\|_2^2 \leq \frac{\left\| W_l^\top w_{l+1} \right\|_2^2}{\left\| (I - V_l V_l^\top)w_{l+1} \right\|_2^2} \leq \frac{\epsilon_{T,T}^{(l)}}{1 - \epsilon_{T,T}^{(l)}} \leq \frac{3}{2} \epsilon_{T,T}^{(l)}.
\]

We will make use of the following lemma from Allen-Zhu and Li (2016) (Lemma B.4).

**Lemma A.1** (Eigen-space perturbation lemma). Let \( M \in \mathbb{R}^{d \times d} \) be a positive semidefinite matrix with eigenvalues \( \lambda_1 \geq \ldots \geq \lambda_r \geq \lambda_{r+1} = \ldots = \lambda_d = 0 \), and corresponding eigenvectors \( u_1, \ldots, u_d \). Define \( U = [u_{j+1}, \ldots, u_r] \in \mathbb{R}^{d \times (r-j)} \) to be the matrix composing of all top \( r \)-eigenvectors with eigenvalues less than or equal to \( \mu \). Let \( v \in \mathbb{R}^d \) be a unit vector such that \( \| U^\top v \|_2 \leq \epsilon \leq 1/2 \), \( v^\top u_{r+1} = \cdots = v^\top u_d = 0 \). Define

\[
\widetilde{M} = (I - vv^\top) M (I - vv^\top).
\]

Denote \( [\widetilde{V}, \widetilde{U}, v, u_{r+1}, \ldots, u_d] \in \mathbb{R}^{d \times d} \) as the orthogonal matrix composed of eigenvectors of \( \widetilde{M} \), where \( \widetilde{U} \) consists of all eigenvectors (other than \( v, u_{r+1}, \ldots, u_d \)) with eigenvalues less than or equal to \( \mu + \tau \). Then there exists a matrix \( Q \) such that \( \| Q \|_2 \leq 1 \) and

\[
\left\| U - \widetilde{U}Q \right\|_2^2 \leq \sqrt{\frac{169 \lambda_1^2 \epsilon^2}{\tau^2} + \epsilon^2}.
\]

By applying Lemma A.1 with \( M = \hat{\Sigma}^{(l)} \),

\[
\widetilde{M} = \hat{\Sigma}^{(l+1)} = (I - v_{l+1}v_{l+1}^\top)\hat{\Sigma}^{(l)}(I - v_{l+1}v_{l+1}^\top), \quad r = d - l, \quad V = W_l, \quad \widetilde{V} = W_{l+1}, \quad v = v_{l+1}, \quad \mu = (1 - \delta + \tau_l) \hat{\mu}, \quad \tau = (\tau_{l+1} - \tau_l) \hat{\mu},
\]

we obtain a matrix \( \widetilde{Q}_l \) such that \( \left\| \widetilde{Q}_l \right\|_2 \leq 1 \) and

\[
\left\| W_l - W_{l+1} \widetilde{Q}_l \right\|_2 \leq \sqrt{\frac{507 \lambda_1^2 \epsilon_{T,T}^{(l)} \mu^2}{2(\tau_{l+1} - \tau_l)^2} + \frac{3}{2} \epsilon_{T,T}^{(l)}} \leq \frac{32 \lambda_1 L}{\lambda_1 \delta}. \]
This inequality combined with inequality (40) together implies
\[
\left\| W_{l+1} \tilde{Q}_l Q_l - \tilde{U} \right\|_2 \leq \left\| W_{l+1} \tilde{Q}_l Q_l - W_l Q_l \right\|_2 + \left\| W_l Q_l - \tilde{U} \right\|_2 \\
\leq \varepsilon_l + \frac{32 \lambda_1 L \sqrt{\varepsilon_T}}{\hat{\lambda}_L \delta}.
\]

By defining \( Q_{l+1} = \tilde{Q}_l Q_l \), we obtain
\[
\left\| \tilde{U} - W_{l+1} Q_{l+1} \right\|_2 \leq \varepsilon_{l+1} : = \varepsilon_l + \frac{32 \lambda_1 L \sqrt{\varepsilon_T}}{\hat{\lambda}_L \delta} = \ldots \\
= \sum_{k=0}^{l+1} \frac{32 \lambda_1 L \sqrt{\varepsilon_T}}{\hat{\lambda}_L \delta} \\
\leq (l + 1) \frac{32 \lambda_1 L \sqrt{\varepsilon_T}}{\hat{\lambda}_L \delta} \\
\leq (l + 1) \frac{32 \lambda_1 L \sqrt{\varepsilon_T}}{\hat{\lambda}_L \delta} \sqrt{\left( \frac{128 \eta^2}{\delta^2 \lambda_k^2} \right)^T} + \frac{512 \eta}{1 - 128 \eta^2 / (\delta \hat{\lambda}_k)^2} \left( \frac{4 \kappa_2^2}{\eta^2} \right)^T,
\]
for \( l = 0, 1, \ldots, L \).

\[
\square
\]

**Appendix B  Proofs of Distributed PCR**

**Proof of Proposition 4.2**

*Proof.* First, notice that
\[
\left\| \hat{\beta} - \beta^* \right\|_2 = \left\| \hat{U}_L O O^\top \hat{\gamma} - U_L \gamma^* \right\|_2 \\
= \left\| \hat{U}_L O O^\top \hat{\gamma} - \hat{U}_L O \gamma^* + \hat{U}_L O \gamma^* - U_L \gamma^* \right\|_2 \\
\leq \left\| O^\top \hat{\gamma} - \gamma^* \right\|_2 + \left\| \gamma^* \right\|_2 \left\| \hat{U}_L O - U_L \right\|_2,
\]
for any orthogonal matrix \( O \).

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Now consider the first part on the RHS.

\[
\|O^\top \hat{\gamma} - \gamma^*\|_2 = \left\| O^\top \left( \tilde{A}^\top \tilde{A} \right)^{-1} \tilde{A}^\top \left( A (U_L - \tilde{U}_L O) \gamma^* + \epsilon \right) \right\|_2 \\
\leq \left\| \left( \tilde{A}^\top \tilde{A} \right)^{-1} \tilde{A}^\top \epsilon \right\|_2 + \left\| \left( \tilde{A}^\top \tilde{A} \right)^{-1} \tilde{A}^\top A \right\|_2 \left\| \left( U_L - \tilde{U}_L O \right) \gamma^* \right\|_2 \\
\leq \left\| \left( \tilde{A}^\top \tilde{A} \right)^{-1} \tilde{A}^\top \epsilon \right\|_2 + \left\| \left( U_L - \tilde{U}_L O \right) \gamma^* \right\|_2.
\]

(42)

Therefore, plug inequality (42) into inequality (41), and notice that \( \|\beta^*\|_2 = 1 \) implies \( \|\gamma^*\|_2 = 1 \), we have

\[
\|\hat{\beta} - \beta^*\|_2 \leq \left\| \left( \tilde{A}^\top \tilde{A} \right)^{-1} \tilde{A}^\top \epsilon \right\|_2 + 2 \left\| \hat{U}_L O - U_L \right\|_2
\]

(43)

By Theorem 2 in Yu et al. (2014), there exists a \( L \times L \) orthogonal matrix \( O \) such that

\[
\left\| \hat{U}_L O - U_L \right\|_F \leq 2^{3/2} \frac{\|\hat{\Sigma} - \Sigma\|_F}{\lambda_L - \lambda_{L+1}}.
\]

(44)

By Corollary 5.50 in Vershynin (2012), with probability at least \( 1 - 2e^{-d\sigma_2^2/C_1} \),

\[
\left\| \hat{\Sigma} - \Sigma \right\|_F \leq \sqrt{\frac{d}{n}} \sigma_2,
\]

(45)

where \( C_1 \) is a constant which only depends on the sub-Gaussian norm of the random vector \( a \).

Also,

\[
\left\| \left( \tilde{A}^\top \tilde{A} \right)^{-1} \tilde{A}^\top \epsilon \right\|_2 \leq \left\| \frac{\tilde{A}^\top \tilde{A}}{n} \right\|^{-1}_2 \left\| \frac{\tilde{A}^\top \epsilon}{n} \right\|_2 = \frac{1}{\lambda_L^{-1}} \left\| \frac{\tilde{A}^\top \epsilon}{n} \right\|_2.
\]

Denote \( \xi = \frac{\tilde{A}^\top \epsilon}{n} \). Notice that \( \xi \) is a \( d \)-dimension sub-Gaussian vector with variance proxy \( \sigma_n^2 \). Therefore, with probability \( 1 - e^{-C_2^2} \)

\[
\|\xi\|_2 = \sqrt{\sum_{i=1}^{d} \xi_i^2} \leq \sqrt{2C_0 \sigma_1} \sqrt{\frac{d}{n}}
\]

. Thus we have,

\[
\left\| \left( \tilde{A}^\top \tilde{A} \right)^{-1} \tilde{A}^\top \epsilon \right\|_2 \leq \sqrt{2} \frac{1}{\lambda_L^{-1}} C_0 \sigma_1 \sqrt{\frac{d}{n}}.
\]

(46)

Combine inequality (44), (45) with inequality (46) we obtain the desired result.
Proof of Theorem 4.3

We define the following matrix, $F$,

$$F = QV_L^\top \hat{U}_L - I_L,$$

where $Q$ is an orthogonal matrix satisfies,

$$Q \triangleq \arg \min_{P : P^\top P = I_L} \|PV_L^\top \hat{U}_L - I_L\|_2.$$

Let $f = \|F\|_2$. Notice that $f$ and $g = \|G\|_2$ are two different error measurements quantifying the estimation error between some estimator $V_L$ and the full covariance estimator $\hat{U}_L$.

Our first lemma discusses the relation between $f$ and $g$.

Lemma B.1. If $\|F\|_2 \leq \varepsilon$, for some $\varepsilon \in [0, 1)$, then $\|G\|_2 \leq \sqrt{2\varepsilon}$. Conversely, if $\|G\|_2 \leq \varepsilon$, for some $\varepsilon \in [0, 1)$, then $\|F\|_2 \leq \varepsilon$. Further, $\|F\|_2 = 0$ if and only if $\|G\|_2 = 0$.

Proof. Note that

$$\|F\|_2 = \|QV_L^\top \hat{U}_L - I_L\|_2 = \|V_L^\top \hat{U}_L Q - I_L\|_2 \leq \varepsilon,$$

which implies that the smallest singular value of $V_L^\top \hat{U}_L Q$ is at least $1 - \varepsilon > 0$. This lower bound combined with $\|Q\|_2 = 1$ implies the smallest singular value of $V_L^\top \hat{U}_L$ is at least $1 - \varepsilon$. Therefore,

$$V_L^\top \hat{U}_L V_L \succeq (1 - \varepsilon)^2 I_L,$$

where $I_L$ is the $L \times L$ identity matrix. Then we have,

$$V_L^\top \hat{U}_L^\top V_L = V_L^\top \left( I_p - \hat{U}_L \hat{U}_L^\top \right) V_L \preceq 2\varepsilon I_L,$$

which implies $\|G\|_2 = \|V_L^\top \hat{U}_L^\top V_L\|_2 \leq \sqrt{2\varepsilon}$.

On the other hand, if $\|G\|_2 \leq \varepsilon$, for some $\varepsilon \in [0, 1)$. Then, we have

$$V_L^\top \hat{U}_L^\top V_L \preceq \varepsilon^2 I_L.$$
Thus,

\[ V_L^\top \hat{U}_L \hat{U}_L^\top V_L = V_L^\top \left( I_d - \hat{U}_L \hat{U} - L \right) V_L \geq (1 - \varepsilon^2) I_L, \]

which implies that the smallest singular value of \( V_L^\top \hat{U}_L \) is at least \( \sqrt{1 - \varepsilon^2} > 0 \). Note that

\[
\left\| Q V_L^\top \hat{U}_L - I_L \right\|_2 = \min_{P: P^\top P = I_L} \left\| PV_L^\top \hat{U}_L - I_L \right\|_2.
\]

Let \( \tilde{Q} = AB^\top \), where \( V_L^\top \hat{U}_L = BDA^\top \) is the SVD of \( V_L^\top \hat{U}_L \). Thus,

\[
\left\| Q V_L^\top \hat{U}_L - I_L \right\|_2 \leq \left\| AB^\top BDA^\top - I_L \right\|_2 = \left\| D - I_L \right\|_2 \leq 1 - \sqrt{1 - \varepsilon^2} \leq \varepsilon,
\]

which concludes the first part of the lemma. The second part is obvious once we have the above results.

This lemma also implies that \( f \leq g \). We also need a second lemma.

**Lemma B.2.** Define \( \tilde{\Sigma} = \frac{1}{n} \hat{A}^\top \hat{A} \), and let \( \tilde{\lambda}_1 \geq \ldots \geq \tilde{\lambda}_L \) be the eigenvalues of \( \tilde{\Sigma} \). It holds that,

\[
\tilde{\lambda}_L \geq \hat{\lambda}_L - \hat{\lambda}_1 (2f + f^2) - \hat{\lambda}_{L+1} g^2.
\]

**Proof.** First, note that \( \tilde{\Sigma} = V_L^\top \hat{\Sigma} V_L \). In fact it is equivalent for us to consider the eigenvalue of

\[
Q \tilde{\Sigma} Q^\top = Q V_L^\top \hat{U} \hat{D} \hat{U}^\top V_L Q^\top = (I_L + F, G) \hat{D} (I_L + F, G)^\top.
\]

Let \( \hat{D}_L = \text{diag} \left( \hat{\lambda}_1, \ldots \hat{\lambda}_L \right) \) and \( \hat{D}_{-L} = \text{diag} \left( \hat{\lambda}_{L+1}, \ldots \hat{\lambda}_n \right) \), and \( \hat{D}_{-L} = \text{diag} \left( \hat{\lambda}_{L+1}, \ldots \hat{\lambda}_n \right) \), then

\[
Q \tilde{\Sigma} Q^\top = \hat{D}_L + \left( F \hat{D}_L + \hat{D}_L F^\top + F \hat{D}_L F^\top + G \hat{D}_{-L} G^\top \right).
\]

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Thus,

\[
\lambda_{\text{min}} \left( Q \tilde{\Sigma} Q^\top \right) \geq \tilde{\lambda}_L - \left\| E \hat{D}_L + \hat{D}_L E^\top + E \hat{D}_L E^\top + F \hat{D}_L F^\top \right\|_2 \\
= \tilde{\lambda}_L - \tilde{\lambda}_1 (2f + f^2) - \tilde{\lambda}_{L+1} g^2
\]

Now we come back to the proof of the theorem.

*Proof.* Similar with the proof of Theorem 4.2, we have

\[
\left\| \tilde{\beta} - \beta^* \right\|_2 \leq \left\| \hat{O}^\top \tilde{\gamma} - \gamma^* \right\|_2 + \left\| \gamma^* \right\|_2 \left\| \hat{V}_L \hat{O} - U_L \right\|_2. \tag{48}
\]

Note that for any orthogonal matrix \( O \), denote \( \hat{O} = Q^\top O \) and

\[
\hat{O}^\top \tilde{\gamma} = ((A V_L \hat{O})^\top A V_L \hat{O})^{-1} (A V_L \hat{O})^\top (A U_L \gamma^* + \epsilon). \tag{49}
\]

From previous proof, We also have

\[
\left\| \hat{O}^\top \tilde{\gamma} - \gamma^* \right\|_2 \leq \left\| \hat{A}^\top \hat{A} \right\|_2 \left\| A \epsilon \right\|_2 + \left\| \hat{A}^\top \hat{A} \right\|_2 \left\| (U_L - V_L \hat{O}) \gamma^* \right\|_2.
\]

Notice that

\[
\left\| \hat{A}^\top \hat{A} \right\|_2 = \left\| \hat{V}_L \hat{U} \hat{D} \hat{U}^\top \hat{V}_L \right\|_2 \leq \left\| \hat{D}_L + F \hat{D}_L + \hat{D}_L F^\top + F \hat{D}_L F^\top + G \hat{D}_L G^\top \right\|_2^{-1} \left\| \hat{D}_L + F \hat{D}_L, G \hat{D}_L \right\|_2 \leq 1 + \left( \tilde{\lambda}_L - \tilde{\lambda}_1 (2f + f^2) - \tilde{\lambda}_{L+1} g^2 \right)^{-1} \left( \tilde{\lambda}_1 (f^2 + f) + \tilde{\lambda}_{L+1} (g^2 + g) \right) \leq 1 + \mu^{-1} \nu. \tag{50}
\]

Combine with equality (49), we have

\[
\left\| \tilde{\beta} - \beta^* \right\|_2 \leq \left\| \hat{A}^\top \hat{A} \right\|_2 \left\| \epsilon \right\|_2 + (2 + \mu^{-1} \nu) \left\| \gamma^* \right\|_2 \left\| \hat{V}_L \hat{O} - U_L \right\|_2 \leq \mu^{-1} \left\| \hat{A}^\top \hat{A} \right\|_2 \left\| \epsilon \right\|_2 + (2 + \mu^{-1} \nu) \left\| \hat{V}_L \hat{O} - U_L \right\|_2.
\]

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Since we can write
\[ \| V_L \hat{O} - U_L \|_2 \leq \| \hat{U}_L O - U_L \|_2 + \| \hat{U}_L - V_L Q^\top \|_2, \]
and
\[ \left( \hat{U}_L - V_L Q^\top \right)^\top \left( \hat{U}_L - V_L Q^\top \right) = -F - F^\top. \]
Thus,
\[ \| V_L \hat{O} - U_L \|_2 \leq \| \hat{U}_L O - U_L \|_2 + \sqrt{2f} \leq \| \hat{U}_L O - U_L \|_2 + \sqrt{2g}. \]

Combining above results and proof from previous section, we complete the proof. \( \square \)

**Appendix C  Proofs of Distributed Gaussian SIM**

**Proof of Theorem 4.6**

We will need a definition on Orlicz norm from Ledoux and Talagrand (2013), in order to deal with random variables whose tail is heavier than sub-Exponential variables.

**Definition C.1.** For \( 1 \leq \alpha < \infty \), let \( \psi_\alpha = \exp(x^\alpha) - 1 \). For \( 0 < \alpha < 1 \), let \( \psi_\alpha(x) = \exp(x^\alpha) - 1 \) for large enough \( x \geq x_\alpha \) and \( \psi_\alpha \) is linear in \( [0, x_\alpha] \) in order to remain global convexity. The Orlicz norm \( \psi_\alpha \) of a random variable \( X \) is defined as
\[ \|X\|_{\psi_\alpha} \triangleq \inf \{ c \in (0, \infty) | \mathbb{E}[\psi_\alpha(|X|/c) \leq 1] \}. \]

**Proof.** Denote \( \Sigma = \mathbb{E}[y (aa^\top - I_d)] \), \( \hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n y_i \cdot (a_i a_i^\top - I_p) \). We first obtain a high probability bound on \( \| \hat{\Sigma} - \Sigma \|_2 \).

Without loss of generality, we can assume \( M = 1 \), otherwise we can always multiply \( M \)
on the bound we obtain. Note that
\[
\left\| \hat{\Sigma} - \Sigma \right\|_2 \leq \frac{1}{n} \sum_{i=1}^{n} y_i (a_i a_i^\top - I_p) - \mathbb{E}[f(\langle \beta^*, a_i \rangle) (aa^\top - I_d)] \leq \frac{1}{n} \sum_{i=1}^{n} f(\langle \beta^*, a_i \rangle) (a_i a_i^\top - I_p) - \mathbb{E}[f(\langle \beta^*, a_i \rangle) (aa^\top - I_d)] + \frac{1}{n} \sum_{i=1}^{n} \epsilon_i (a_i a_i^\top - I_d).
\]

Under Lemma 5.4 in Vershynin (2012), We can evaluate the operator norm on the RHS of inequality (51) on a $\frac{1}{4}$-net $\mathcal{E}$ of the unit sphere $S^{d-1}$:
\[
\left\| \frac{1}{n} \sum_{i=1}^{n} f(\langle \beta^*, a_i \rangle) (a_i a_i^\top - I_p) - \mathbb{E}[f(\langle \beta^*, a_i \rangle) (aa^\top - I_d)] \right\|_2 \leq 2 \max_{v \in \mathcal{E}} \left| \frac{1}{n} \sum_{i=1}^{n} f(\langle \beta^*, a_i \rangle) (z(v)^2 - 1) - \mathbb{E}[f(\langle \beta^*, a_i \rangle) (z(v)^2 - 1)] \right|
\]
where $z(v) = v^\top a \sim \mathcal{N}(0, 1)$. Notice that $z(v)^2 - 1$ is a sub-Exponential with parameter $(2, 4)$, and $\mathbb{E}\{f(\langle \beta^*, a \rangle) (z(v)^2 - 1)\} \geq -2$. Therefore, denote $\theta = \max\{1, 2M\}$, $\forall |s| \leq \frac{1}{8\theta}$,
\[
\mathbb{E} \left[ \exp\{s(\langle \beta^*, a \rangle) (z(v)^2 - 1) - \mathbb{E}[f(\langle \beta^*, a \rangle) (z(v)^2 - 1))\] \leq 1 + \sum_{k=2}^{\infty} \frac{|s|^k}{k!} \mathbb{E} \left| f(\langle \beta^*, a \rangle) (z(v)^2 - 1) - \mathbb{E} (f(\langle \beta^*, a \rangle) (z(v)^2 - 1)) \right|^k \leq 1 + \sum_{k=2}^{\infty} \frac{|s|^k}{k!} 2^k \mathbb{E} \left| (z(v)^2 - 1) \right|^k \leq 1 + \sum_{k=2}^{\infty} \frac{|s|^k}{k!} (2M)^k \mathbb{E} \left| (z(v)^2 - 1) \right|^k \leq 1 + \sum_{k=2}^{\infty} (|s|^k 8M)^k \leq \exp\{s^2(16M)^2/2\}.
\]
Thus, $\tilde{X} \triangleq f(\langle \beta^*, a \rangle) (z(v)^2 - 1)$ is a sub-Exponential with parameter $(16M, 8\theta)$. Therefore, by Proposition 5.16 in Vershynin (2012), we can obtain a Bernstein-type inequality:
\[
\mathbb{P} \left[ \left| \frac{1}{n} \sum_{i=1}^{n} \tilde{X}_i - \mathbb{E} \tilde{X} \right| > 8\theta \epsilon \right] \leq 2 \exp \left[ -\frac{n}{2} (\epsilon^2 \land \epsilon) \right],
\]
for any \( \epsilon > 0 \). Now let \( \epsilon = \max(\gamma, \gamma^2) \), where \( \gamma = C \sqrt{\frac{d}{n}} + \frac{\delta_1}{\sqrt{n}} \), for some constant \( C \) and \( \delta_1 > 0 \). Now we have,

\[
P \left( \left| \frac{1}{n} \sum_{i=1}^{n} \tilde{X}_i - \mathbb{E} \tilde{X} \right| > 80\gamma \right) \leq 2 \exp \left( -\frac{n}{2} \gamma^2 \right) \leq 2 \exp \left( -\frac{1}{2} (C^2 d + \delta_1^2) \right).
\]

Notice that by Lemma 5.2 in Vershynin (2012), we can choose the net \( \mathcal{E} \) so that it has cardinality \( |\mathcal{E}| \leq 9^d \). Therefore, we take the union bound over all vectors \( \mathbf{v} \in \mathcal{E} \), we obtain

\[
P \left( \max_{\mathbf{v} \in \mathcal{E}} \left| \frac{1}{n} \sum_{i=1}^{n} \tilde{X}_i - \mathbb{E} \tilde{X} \right| > 80\gamma \right) \leq 2 \times 9^d \exp \left( -\frac{1}{2} (C^2 d + \delta_1^2) \right) = 2 \exp \left( -\frac{\delta_1^2}{2} \right), \tag{52}
\]

where we can choose \( C \) sufficiently large, e.g. \( C = 2\sqrt{\ln 3} \).

For the second part on the RHS of the inequality (51), we have

\[
\left\| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i (a_i a_i^\top - I_d) \right\|_2 \leq \left\| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i a_i a_i^\top \right\|_2 + \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i \right|.
\]

Given that \( \epsilon \)s are independent sub-Gaussian(\( \sigma \)) random variables with mean 0, we have

\[
\left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i \right| \leq \sigma \delta_2 \frac{1}{\sqrt{n}}, \tag{53}
\]

with probability at least \( 1 - 2 \exp(-\delta_2^2/2) \).

Now, in order to control \( \left\| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i a_i a_i^\top \right\|_2 \), we consider \( \left\| \sum_{i=1}^{n} \mathbb{E} \| a_i \|_2^2 a_i a_i^\top \right\|_2 \) first. Under a \( \frac{1}{4} \)-net \( \mathcal{E}_2 \) of the unit sphere \( S^{d-1} \),

\[
\left\| \sum_{i=1}^{n} \| a_i \|_2^2 a_i a_i^\top - \mathbb{E} \left\| \sum_{i=1}^{n} \mathbb{E} \| a_i \|_2^2 a_i a_i^\top \right\|_2 \right\|_2 \leq 2 \max_{\mathbf{v} \in \mathcal{E}_2} \sum_{i=1}^{n} \| a_i \|_2^2 (\mathbf{v}^\top a_i)^2 - \mathbb{E} \sum_{i=1}^{n} \| a_i \|_2^2 (\mathbf{v}^\top a_i)^2
\]

\[
= 2 \max_{\mathbf{v} \in \mathcal{E}_2} \sum_{i=1}^{n} \| a_i \|_2^2 (\mathbf{v}^\top a_i)^2 - \mathbb{E} \sum_{i=1}^{n} \| a_i \|_2^2 (\mathbf{v}^\top a_i)^2
\]

\[
= 2 \max_{\mathbf{v} \in \mathcal{E}_2} \sum_{i=1}^{n} \sum_{j=1}^{d} a_{ij}^2 z(\mathbf{v})_i^2 - \mathbb{E} \sum_{i=1}^{n} \sum_{j=1}^{d} a_{ij}^2 z(\mathbf{v})_i^2,
\]

where \( a_{ij} \sim \mathcal{N}(0, 1) \) is the \( j \)-th term of \( a_i \) and \( z(\mathbf{v})_i = \mathbf{v}^\top a_i \sim \mathcal{N}(0, 1) \). Notice that \( a_{ij}^2, z(\mathbf{v})_i^2 \sim \chi^2(1) \), and

\[
P(a_{ij}^2 z(\mathbf{v})_i^2 \geq t) \leq P(a_{ij}^2 \geq \sqrt{t}) + P(z(\mathbf{v})_i^2 \geq \sqrt{t}) \leq 2 \exp(-\sqrt{t}/2),
\]

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for all $i \in \{1, \ldots, n\}, j \in \{1, \ldots, d\}$. Therefore, denote

$$\|a_{ij}^2z(v)^2\|_{\psi_{1/2}} \leq K_\psi,$$

where $K_\psi$ is a finite constant. By Theorem 8.4 in Ma and Wigderson (2015), there exists a constant $K_\alpha$ such that

$$\left\| \sum_{i=1}^{n} \sum_{j=1}^{d} a_{ij}^2 z(v)^2 - E \sum_{i=1}^{n} \sum_{j=1}^{d} a_{ij}^2 z(v)^2 \right\|_{\psi_{1/2}} \leq K_\alpha K_\psi \sqrt{nd \log(nd)}.$$

Denote $Z = \sum_{i=1}^{n} \sum_{j=1}^{d} a_{ij}^2 z(v)^2 - E \sum_{i=1}^{n} \sum_{j=1}^{d} a_{ij}^2 z(v)^2$ and $K_Z = \left\| \sum_{i=1}^{n} \sum_{j=1}^{d} a_{ij}^2 z(v)^2 - E \sum_{i=1}^{n} \sum_{j=1}^{d} a_{ij}^2 z(v)^2 \right\|_{\psi_{1/2}}$. Using Markov inequality, we have

$$P(|Z| > t) \leq \frac{E\left[\psi_{1/2}(Z/K_Z) + 1\right]}{\psi_{1/2}(t/K_Z) + 1} \leq 2 \exp \left\{ - \left( \frac{t}{K_Z} \right) \right\}.$$

By a union bound, we have

$$P \left[ \left\| \sum_{i=1}^{n} \|a_i\|_2^2 a_i a_i^T - E \sum_{i=1}^{n} \|a_i\|_2^2 a_i a_i^T \right\|_2 \geq t \right] \leq 2 \times 9^d \exp \left\{ - \left( \frac{t}{K_Z} \right) \right\}.$$

Therefore, with probability at least $1 - 2 \exp(-\delta_3)$,

$$\left\| \sum_{i=1}^{n} \|a_i\|_2^2 a_i a_i^T - E \sum_{i=1}^{n} \|a_i\|_2^2 a_i a_i^T \right\|_2 \leq 5K_\alpha K_\psi \sqrt{nd \log(nd)d^2} + \delta_3 K_\alpha K_\psi \sqrt{nd \log(nd)}.$$

Note that

$$\left\| E \sum_{i=1}^{n} \|a_i\|_2^2 a_i a_i^T \right\|_2 \leq n \left\| E \|a_i\|_2^2 a_i a_i^T \right\|_2 \leq 3nd.$$

Thus, with probability at least $1 - 2 \exp(-\delta_3)$,

$$\left\| \sum_{i=1}^{n} \|a_i\|_2^2 a_i a_i^T \right\|_2 \leq 5K_\alpha K_\psi \sqrt{nd \log(nd)d^2} + \delta_3 K_\alpha K_\psi \sqrt{nd \log(nd)} + 3nd \leq 10K_\alpha K_\psi \sqrt{nd \log nd^2} + 2\delta_3 K_\alpha K_\psi \sqrt{nd \log n} + 3nd.$$

By Theorem 4.1.1 in Tropp et al. (2015),

$$P \left( \left\| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i a_i a_i^T \right\|_2 \geq t \right) \leq 2d \exp \left\{ - \frac{t^2}{2 \left\| \frac{1}{n} \sum_{i=1}^{n} \|a_i\|_2^2 a_i a_i^T \right\|_2} \right\},$$

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which yields that with a probability over \(1 - 2 \exp(-\delta_3) - 2 \exp(-\delta_4)\),

\[
\left\| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i a_i a_i^\top \right\|_2 \leq \sqrt{2 \ln d} \left\| \frac{1}{n^2} \sum_{i=1}^{n} a_i a_i^\top \right\|_2 + \sqrt{\delta_4} \left\| \frac{1}{n^2} \sum_{i=1}^{n} \epsilon_i a_i a_i^\top \right\|_2 \\
\leq \left( \sqrt{\delta_4 d + \sqrt{d \log d}} \right) \left( \frac{(20 + 4\delta_3^2)K\psi d \sqrt{d \log n}}{\sqrt{n}} \right) + \frac{8\delta_1 + \sigma\delta_2}{\sqrt{n}}.
\]

where we use Assumption 4.5. Combine inequality (51), (52), (53) as well as inequality (54), we have with probability at least \(1 - 2 \exp(-\delta_1^2/2) - 2 \exp(-\delta_2^2/2) - 2 \exp(-\delta_3) - 2 \exp(-\delta_4)\),

\[
\left\| \hat{\Sigma} - \Sigma \right\|_2 \leq 17\theta \sqrt{\frac{d}{n}} + \sqrt{(20 + 4\delta_3^2)K\psi C \delta_4} + \frac{8\delta_1 + \sigma\delta_2}{\sqrt{n}} + \frac{d \sqrt{\log d \log n}}{\sqrt{n}}.
\]

By Corollary 3.1 in Vu et al. (2013),

\[
\min_{t \in \{-1,+1\}} \|t\hat{\beta} - \beta^*\|_2 = \min_{t \in \{-1,+1\}} \sqrt{2} \left\| \Theta(t\hat{\beta}, \beta^*) \right\|_F \leq 2 \left\| \hat{\Sigma} - \Sigma \right\|_2.
\]

Combine bound (56) with (55), we have the desired result. \(\square\)

### Appendix D Additional Experiments

In this section, we present the experimental results on distributed PCR and distributed Gaussian SIM.

#### Numerical results of distributed PCR

We provide numerical results of distributed PCR in this section. Recall the problem setting in Section 4.1. We assume the real coefficient \(\beta^*\) lies in the top-3-dim eigenspace of \(\Sigma\), i.e., \(\beta^* = U_3 \gamma^*\), where \(U_3 = [u_1, u_2, u_3]^\top\) consists of the top-3 eigenvectors of \(\Sigma\). As in previous experiments, data dimension \(d\) is set to 50, and sample size on each machine is 52.
set to 500, i.e., \( a \in \mathbb{R}^{50} \), \( m = 500 \). We vary the the number of machines. The response vector \( y \in \mathbb{R}^{mK} \) is generated by \( y = A\beta^* + \epsilon \), where noise term \( \epsilon \sim \mathcal{N}(0, \sigma^2 I_{mK}) \), and \( \sigma^2 \) is a constant, which is set to 0.2 and 0.5 in the following experiments. Here covariate data matrix \( A = [a_1, \ldots, a_{mK}]^\top \in \mathbb{R}^{mK \times d} \) is drawn i.i.d. from \( \mathcal{N}(0, \Sigma) \) with \( \Sigma = U\Lambda U^\top \), \( \Lambda = \text{diag}(2.5, 2, 1.5, 1, \ldots, 1) \). \( \gamma \) is sampled only once from \( \mathcal{N}(0, I_3) \) and is fixed in our 100 Monte-Carlo simulations. Moreover, the underlying true regression coefficient is \( \beta^* = U_3 \frac{\gamma}{\|\gamma\|_2} \).

We estimate \( U_3 \) using 3 different estimation methods and compare their performances. The measurement we use here is the \( l_2 \) distance between estimator \( \hat{\beta} \) and real coefficient \( \beta^* \), i.e., \( \text{error}(\hat{\beta}) = \|\hat{\beta} - \beta^*\|_2 \). The numbers of outer iterations and inner iterations in our algorithm are fixed as 40 and 10, respectively. The results are shown in Figure D.5. In accordance with previous experiments, our method almost keeps the same error rate as the oracle one.

Figure D.5: Comparison between algorithms in PCR when the number of machines varies. The x-axis is the the number of machines and the y-axis is the log-\( l_2 \) error. On the left, the noise term has variance 0.2 and on the right figure, 0.5.
Numerical results of distributed SIM

In our last part of the experiments, we conduct simulations on Gaussian single index model. Consider data dimension $d$ to be 50, sample size on each machine to be 500, i.e., $\mathbf{a} \in \mathbb{R}^{50}$, $m = 500$. Our covariate data matrix $\mathbf{A} \in \mathbb{R}^{mK \times d}$ is drawn independently, where each row $\mathbf{a}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$ follows a standard normal distribution. For the data generating process of $\mathbf{y} = (y_1, \ldots, y_{mK})^\top \in \mathbb{R}^{mK}$, we have $y_i = f(\langle \beta^*, \mathbf{a}_i \rangle) + \epsilon_i$, $\forall i \in \{1, \ldots, mK\}$, where $f(\cdot)$ is our specific choice of link function, $\beta^*$ is a normalized vector only drawn once during Monte-Carlo process from $\mathcal{N}(\mathbf{0}, \mathbf{I}_d)$, i.e., $\beta^*/\|\beta\|_2$, $\beta \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$ and $\{\epsilon_i\}$ are i.i.d. normal $\mathcal{N}(\mathbf{0}, \sigma^2)$ with the constant variance $\sigma^2$ fixed to be 0.2. During our estimation process, we estimate top eigenvector $\hat{\beta}$ of $\frac{1}{mK} \sum_{i=1}^{mK} y_i \cdot (\mathbf{a}_i \mathbf{a}_i^\top - \mathbf{I}_d)$.

In the following experiment, we consider three different link functions: $f(u) = u^2, f(u) = |u|$ and $f(u) = 4u^2 + 3 \cos(u)$. The $l_2$ distance $\|\hat{\beta} - \beta^*\|_2$ is used here to measure the performance. In Figure D.6, for all choices of link function, our estimators have the same errors as the oracle results. For this experiment, the DC method also works well, which is mainly because the problem of estimating the top eigenvector is relatively simple and $\mathbf{a}$ follows a symmetric normal distribution.