One-shot Distributed Algorithm for PCA with RBF Kernels

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Abstract—This letter proposes a one-shot algorithm for feature-distributed kernel PCA. Our algorithm is inspired by the dual relationship between sample-distributed and feature-distributed scenario. This interesting relationship makes it possible to establish distributed kernel PCA for feature-distributed cases from ideas in distributed PCA in sample-distributed scenario. In theoretical part, we analyze the approximation error for both linear and RBF kernels. The result suggests that when eigenvalues decay fast, the proposed algorithm gives high quality results with low communication cost. This result is also verified by numerical experiments, showing the effectiveness of our algorithm in practice.

Index Terms—Distributed data, distributed learning, principal component analysis, one-shot algorithm, RBF kernels.

I. INTRODUCTION

P RINCIPAL Component Analysis (PCA) is a fundamental technology in machine learning. For nonlinear tasks, PCA could be formulated as the following problem,

$$\max_{w, w=1} \|w^T \phi(X)\|^2_F.$$  \hspace{1cm} (1)

Here $X \in \mathbb{R}^{M \times T}$ denotes data and $\phi(\cdot) : \mathbb{R}^M \rightarrow \mathcal{F}$ is a unknown non-linear mapping. Interestingly, the kernel trick could be implemented there, resulting the kernel PCA (KPCA) [1][2][3]. Specifically, the optimal solution of (1) is $w = \phi(X)\alpha$, where $\alpha$ is the eigenvectors of the gram kernel matrix $K \triangleq \langle \phi(X), \phi(X) \rangle$.

Nowadays, distributed algorithm of KPCA is in high demand. Generally, distributed data could be categorised as two regimes, namely horizontally and vertically partitioned data [4][5]. As shown in Fig. 1, the horizontal and vertical axes are features and samples. Then, when data are partitioned horizontally, agents contain part of samples with all features; when data are partitioned vertically, agents contain full samples but with only part of features.

For PCA problems, there are massive researches focusing on both the horizontal [3][6][7] and the vertical regime [8][9][10]. However, although KPCA are very common in practice, e.g., in face recognition [11, 12] and process monitoring [13, 14], applicable distributed algorithms are not much. To the best of our knowledge, the existing studies on distributed KPCA are all for the horizontal regime, most of which require multi-communication rounds; see, e.g., [13][16][17].

In this letter, we aim to develop distributed KPCA for vertically partitioned data. The main obstacle in vertical regime is that we only locally know a part of features, then it seems that one cannot know the global kernel without heavy communication. To handle this problem, we fully investigate the kernel trick that can transfer the primal optimization variables corresponding to features to dual variables corresponding to samples. With this idea, we can link KPCA in the vertical regime to PCA in the horizontal regime and establish a distributed KPCA (DKPCA) in the vertical regime. The proposed DKPCA locally calculates the the first $D$ eigenvectors and their corresponding eigenvalues of local kernel matrices and then sent to a fusion center, where they are aggregated to reproduce local estimators. DKPCA is applicable to both linear and RBF kernel and it needs only one communication round. Theoretical discussion will show that the approximation error is related to the $D$-th eigenvalue of local matrices. When eigenvalues decay fast, DKPCA has very high quality results, which is also confirmed by numerical experiments.

II. DISTRIBUTED KERNEL PCA

A. Preliminaries and Notations

We use regular letters for scalars, capital letters in bold for matrices and lowercase letters in bold for vectors. For a matrix $A$, $\|A\|_F$ represents the Frobenius norm. We consider a distributed setting, where the data are partitioned vertically and stored distributedly in $J$ local agents. Such vertical regime are common in practice, e.g., in wireless sensor networks [18][19], ranking or evaluation systems [20][21]. Specifically, each agent $j$ acquires a zero-mean data vector $x^{(j)} = \{x_i^{(j)}\}_{i=1}^{M_j} \in \mathbb{R}^{M_j \times T}$, which is i.i.d. at time $i = 1, 2, \cdots, T$. $M_j$ is the feature dimension of the data $x^{(j)}$ and we have $\sum_{j=1}^{J} M_j = M$. Let $X = [(x^{(1)})^T (x^{(2)})^T \cdots (x^{(J)})^T]^T \in \mathbb{R}^{M \times T}$ denote all data collected by agents, which are not stored together but given for convenience.

Fig. 1: Categorizations of data partition in distributed setting.
Here we briefly review the KPCA problem, i.e., problem (1), where PCA is executed in a Reproducing Kernel Hilbert Space (RKHS) introduced by a reproducing kernel $\kappa(\cdot, \cdot)$. The goal of KPCA is to diagonalize the covariance matrix $C = \sum_i \phi(x_i) \otimes \phi(x_i)^\ast$. However, it is hard to do eigendecomposition on $C$ since $\phi$ is implicit. Then KPCA turns to solve the dual eigenproblem, where the eigendecomposition is performed on the gram kernel matrix $K \in \mathbb{R}^{T \times T}$, i.e.,

$$K_{p,q} = \kappa(x_p, x_q) = \langle \phi(x_p), \phi(x_q) \rangle, \quad p, q = 1, \ldots, T,$$

\[ \lambda_d \alpha_d = K \alpha_d, \quad d = 1, \ldots, T, \]

where $\alpha_d \in \mathbb{R}^{T \times 1}$ is the eigenvector of $K$ corresponding to the $d$-th largest eigenvalue $\lambda_d$. Then the $d$-th eigenvector of $C$ can be rewritten as $w_d = \phi(X)\alpha_d$. Such kernel trick sidesteps the problem of computing unknown $\phi(\cdot)$ and moreover, it makes the distributed computation for vertically partitioned data more convenient because:

- the covariance $C$ is not separable and generally the approximation by local covariance matrices is not accurate, e.g., $C \neq \sum_i C^{(i)} = \sum_i \sum_j \phi(x^{(j)}_i) \otimes \phi(x^{(j)}_i)^\ast$.
- $K$ itself (linear kernels) or its main calculation part (RBF kernels) is separable, e.g., a linear kernel $K = \sum_j K^{(j)}$.

**B. Distributed algorithm for kernel PCA**

We first link the existing distributed algorithm for PCA in horizontal regime [5] to that for KPCA in vertical regime, and then extend it to RBF kernels. The proposed algorithm could produce a good estimation to the global optimum in one-communication round with privacy protection.

In the horizontal regime, the key property is the consistency between the sum of local covariance matrices and the global covariance matrix, i.e., $C = \sum_j C_j$, which results in benefits for both algorithm design and theory analysis. Considering linear KPCA in vertical regime is a dual problem of linear KPCA in vertical regime, we can easily transfer the algorithm in [5] to that of KPCA. Mathematically, for linear kernels, $\phi(x) = ax, \forall a \in \mathcal{R}$. We assume $a = 1$ without loss of generality and then it holds that $K = X^\top X = \sum_{j=1}^D (x^{(j)})^\top x^{(j)} = \sum_j K^{(j)}$. Thus, the estimator $\hat{K}$ is calculated as follow.

$$\hat{K} = \sum_j \hat{K}^{(j)} = \sum_j V_D^{(j)} \lambda_D^{(j)} (V_D^{(j)})^\top. \quad (2)$$

However, in horizontal regime, algorithm in [5] cannot be extend to non-linear case, limiting its application in practice.

**Algorithm 1** One-shot distributed algorithm for kernel PCA in the vertical partition regime. (DKPCA)

1. On local agents, calculate the local kernel matrix $K^{(j)}$. Solve eigenvalue problem on $K^{(j)}$, obtaining $V_D^{(j)}$ and $\lambda_D^{(j)}$ and sent them to the fusion center.
2. On the fusion center, calculate $\hat{K}$ to approximate $K$.
   - For linear kernel, use (2).
   - For RBF kernel, use (4).
3. Compute the leading $D$ eigenvectors $\hat{V} \in \mathbb{R}^{T \times D}$ of the approximate matrix $K$.
4. return $\hat{V}$.

Instead, in vertical regime, we can further extend this idea to RBF kernels by noting the following property.

$$K(p, q) = \kappa(x_p, x_q) = \exp \left( -\frac{\|x_p - x_q\|^2}{2\sigma^2} \right)$$

where $\sigma$ is the kernel width. Using $\circ$ to denote the Hadamard (element-wise) product operator, we rewrite $\hat{K}$ as $K = K^{(1)} \circ K^{(2)} \circ \ldots \circ K^{(J)}$. Therefore, once the eigenvectors of each local kernel matrix are obtained, the whole kernel matrix $K$ could be approximated as the following way,

$$\hat{K} = K^{(1)} \circ \ldots \circ K^{(J)}$$

Finally, we compute the first $D$ eigenvectors of $\hat{K}$, denoted as $\hat{V}$, and the projection matrix $\hat{W} = \sum_j V_j \phi(x_j)$. Notice that for this calculation, $\hat{W}$ is unknown but $(\hat{W}, \phi(y))$ can be calculated by kernel trick in a distributed system because $x^\top y$ and $\|x - y\|^2$ is separable along features. The overall algorithm is summarized in Algorithm 1.

**Approximation Analysis.** Here we present the approximation analysis for DKPCA in both linear and RBF cases. Specifically, we study the $\sin \Theta$ distance between the eigenspaces spanned by $V$ and $\hat{V}$, where $V$ are the eigenvectors of the global gram kernel matrix $K$, $\hat{V}$ is the estimator calculated by DKPCA. $\sin \Theta$ distance is well-defined and is widely used for measuring the distance between two linear spaces [5][22]. Let $\alpha_1, \ldots, \alpha_D$ be the singular values of $V^\top \hat{V}$ and define $\sin \Theta(V, \hat{V})$ as follows.

$$\Theta(V, \hat{V}) = \text{diag}\{\cos^{-1}(\alpha_1), \ldots, \cos^{-1}(\alpha_D)\} \triangleq \text{diag}\{\sin(\theta_1), \ldots, \sin(\theta_D)\}. \quad (5)$$

**Theorem 1.** Let $V \in \mathbb{R}^{T \times D}$ be the first $D$ eigenvectors of the global kernel matrix $K \in \mathbb{R}^{T \times T}$ that is derived by a kernel function $\kappa$, and $\hat{V}$ be its approximation computed by DKPCA. If $\kappa$ is a linear kernel, then $V$, $\hat{V}$ satisfy

$$\|\sin \Theta(V, \hat{V})\|_F \leq J \sqrt{T - D} \max_j (\lambda_D^{(j)}). \quad (6)$$

If $\kappa$ is a RBF kernel, then $V$, $\hat{V}$ satisfy

$$\|\sin \Theta(V, \hat{V})\|_F \leq J \sqrt{T \max_j (\lambda_D^{(j)})} \lambda_D - \lambda_{D+1}. \quad (7)$$

See supplemental materials for the proof of Theorem 1. Theorem 1 indicates that the approximation error is related with $J$, $T$, $D$ and $\lambda$. If $\lambda$ decay fast, which is common for RBF kernels, then DKPCA will have very high quality results.

**Communication and Computation cost.** Alg. 1 is quite
TABLE I: Communication and computation complexity of three kinds of algorithms for PCA.

|               | COMM.                | COMP.                |
|---------------|----------------------|----------------------|
| DPDA [5]      | $O((MJ)/M)$          | $O((\max(M,(M/J+D))J)^2)$ |
| DKPCA (Alg. [1]) | $O((J)/T)$          | $O((\max(T,(M(J+D))J)^2)$ |
| KPCA (SVD-based) | $O((TM/J))$          | $O(T^3)$             |

efficient with only one round communication. To analyze quantitatively, we restrict our discussion on the evenly distributed situation, i.e., the local feature dimension is $O(M/J)$ and there is no statistic difference among the nodes. The discussion on other cases is similar but is more complicated in form. We summarize the communication and computation complexity of distributed PCA (DPDA) [5], Alg. [1] and central KPCA in Table I.

Compared with central algorithms, where additional communication and fusion are required, DKPCA sacrifices computation efficiency for communication efficiency. To pursue high communication efficiency, we prefer a small $D$, e.g., when $D$ is much smaller than $M/J$, DKPCA has significant advantage over central algorithms on communication cost. As for the computation cost, for given data, if $T \geq 2\sqrt{M(D+1)}$ and

$$J \in \left[ \frac{T - \sqrt{\Delta}}{2(D+1)}, \frac{T + \sqrt{\Delta}}{2(D+1)} \right]$$

with $\Delta = T^2 - 4M(D+1)$.

Then the computation cost is $O(T^3)$, the same as central algorithms. Notice that the required condition is not strict. For example, if $M = 10000$, $D = 100$, $T = 5000$, then $J \in [3, 47]$, which is a large range, will meet the above requirement such that the computation cost is $O(T^3)$.

**Self-adaptive strategy for data maldistribution.** Herein-before, we simply set equal $D(j)$ in every local agents for DKPCA, which, however, may not work well for the case of data maldistribution. Thm. [1] shows that for given $J, T, \delta$, the error is related to $\delta$ and $\max_j(\lambda_{D+1}^{(j)})$. To reduce the approximate error, small $\lambda_{D+1}^{(j)}$ is preferred. Thus, local agents that have larger eigenvalues (which means they hold more information) need to send more number of eigenvectors. On the other side, in some agents, the eigenvalues decay fast so that the $D$-th one are almost 0. Then sending $D$ eigenvectors is redundant.

Therefore, we consider the following self-adaptive strategy for the selection of $D(j)$ such that each agent can decide the number of the eigenvectors sent to the center according to their local eigenvalues $\lambda_{D}^{(j)}$:

$$D(j) = \min \{ \min_k \{ \lambda_{D+1} \leq \epsilon \}, T \}$$

where $\epsilon$ is a positive threshold value. Note that the decays of $\lambda_{D}$ are generally assumed to be polynomial or exponential \[\lambda_{i} = O(i^{-\rho})\] or $\lambda_{i} = O(e^{-\rho\iota})$. Then the $D$ given by \[(8)\] is $\Omega((\frac{1}{\rho})^{\frac{1}{\rho}})$ or $\Omega(-\frac{1}{\rho} \log(\epsilon))$, where $c$ is some constant.

### III. EXPERIMENTS

The performance of DKPCA is evaluated here by three experiments, where both simulation and real data are used. We will show the different performance of DKPCA for data with different $J, T, \delta$ in section III.
data and the RBF kernel are used with PCA. The aim of PCA is to keep useful information during data projection. Here we will show that DKPCA can preserve similar information as PCA. That is, the same post learning algorithm can achieve similar performance on the two projected data produced by DKPCA and PCA. We first map data into a low-dimension feature space by DKPCA, the central kernel algorithm (KPCA) with RBF kernels with parameters \( \sigma = 50 \), and the central linear algorithm (PCA), for which the corresponding eigenproblems are all solved by SVD. The feature dimension of the projected data changes from 1 to 200. The projected data are then sent as a linear support vector machine (L-SVM). We randomly choose 200 data as the training set and use the rest for test.

The average classification error and its standard deviation over 50 trials are reported in Table II. As the feature dimension of the projected data increases, the classification error rates of all methods decrease. KPCA is based on full data and is expected to be better than the proposed DKPCA. But from Table II, one could observe that the difference is slight. In KPCA and DKPCA, the RBF kernel is applied and thus achieves less classification error than PCA, although the PCA process involves much more calculation. The average communication cost and its standard deviation over 50 trials are reported in Table II. The projected data are then sent as a linear support vector machine (L-SVM). We randomly choose 200 data as the training set and use the rest for test.

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### IV. Conclusion

This letter introduced a one-shot privacy-preserving algorithm, DKPCA, for distributed kernel PCA in vertical regime. The main technique is kernel trick, by which the vertical regime and horizontal regime is linked up and nonlinear dimension reduction could be implemented with RBF kernels. We presented the approximation analysis and experiments result of DKPCA, which coincides with the theoretical result and demonstrate that DKPCA is effective to extract non-linear features and is communication efficient.
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