Distributed Kernel Principal Component Analysis

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Abstract

Kernel Principal Component Analysis (KPCA) is a key technique in machine learning for extracting the nonlinear structure of data and pre-processing it for downstream learning algorithms. We study the distributed setting in which there are multiple servers, each holding a set of points, who wish to compute the principal components of the union of their pointsets. Our main result is a communication and computationally efficient algorithm that takes as input arbitrary data points and computes a set of global principal components with relative-error approximation for polynomial kernels.

While recent work shows how to do PCA in a distributed setting, the kernel setting is significantly more challenging. Although the “kernel trick” is useful for efficient computation, it is unclear how to use it to reduce communication. The main problem with previous work is that it achieves communication proportional to the dimension of the data points, which if implemented straightforwardly in the kernel setting would give communication either proportional to the dimension of the feature space, or to the number of examples, both of which could be very large. We instead take a roundabout approach, using a careful combination of oblivious subspace embeddings for kernels, oblivious leverage score approximation, adaptive sampling, and sketching for low rank approximation to achieve our result. We also show that our algorithm enjoys strong performance on large scale datasets.

1 Introduction

Principal Component Analysis (PCA) is a widely used tool for dimensionality reduction and data preprocessing. It consists of finding the most relevant lower-dimension subspace of the data in the sense that the projection should capture as much of the variance of the original data as possible. Kernel Principal Component Analysis (KPCA) is the extension of this method to data mapped to the kernel feature space [Schölkopf et al., 1997]. It allows one to exploit the nonlinear structure of the data, since the vectors in the kernel feature space correspond to nonlinear functions in the original space. This is crucial for complex data such as text and image data, and thus KPCA finds its application for many learning problems. However, such data sets are often large scale, and KPCA is known to be computationally expensive and not easily scalable.

Since large scale data is often partitioned across multiple servers, there is an increasing interest in solving learning problems in the distributed model. Kernel methods in this setting face an additional subtle difficulty. The algorithm should use the kernel trick to avoid going to the kernel feature space explicitly, so intermediate results are often represented by a function (e.g., a weighted combination) of the feature mapping of some data points. Communicating such intermediate results requires communicating all the data points they depend on. To lower the communication cost, the intermediate results should only depend on a small number of data points. A distributed algorithm then needs to be carefully designed to meet this constraint.

In this paper, we propose a distributed algorithm to compute KPCA for the polynomial kernel. For $n$ data points in $\mathbb{R}^d$ arbitrarily partitioned over $s$ servers, the algorithm computes a rank-$k$ subspace in

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the kernel feature space, which is represented by $O(k/\epsilon)$ original points and achieves a $(1 + \epsilon)$ relative-error approximation compared to the best rank-$k$ subspace. The total communication of the algorithm is $\tilde{O}(sdk/\epsilon + spoly(k/\epsilon))$, which nearly matches $O(sdk/\epsilon)$, the communication of the state-of-the-art algorithms for linear PCA. As far as we know, this is the first algorithm that can achieve relative-error approximation with these communication bounds. It also leads to distributed algorithms for some other kernel methods: the data can then be projected onto the subspace found and processed by downstream non-linear applications. For example, our algorithm combined with any $\alpha$-approximation distributed $k$-means algorithm leads to a $(1 + \epsilon)\alpha$-approximation distributed kernel $k$-means clustering algorithm. An intermediate result in the development of our algorithm that may be of independent interest is a distributed algorithm for approximating statistical leverage scores for polynomial kernels. This is a subroutine in our distributed KPCA algorithm, but it can also be useful for other problems where leverage scores are related. Finally, our method can be viewed as a general framework for distributed kernel PCA. It can be applied to other kernels as long as subspace embedding for the kernel is available; see Section 2.2 for more details.

Experimental results on large scale real world data show that our algorithm can be run on large datasets for which non-distributed algorithms can be prohibitive, and can achieve significantly better error than the baseline with the same communication budget, with running time about twice that of basic approaches on datasets of size smaller by orders of magnitude.

1.1 Overview of Main Results

Suppose there are $s$ servers that are connected to a central processor. Server $i \in [s]$ has a local data set $A^i \in \mathbb{R}^{d \times n_i}$, and the global data set $A \in \mathbb{R}^{d \times n}$ is the union of the local data ($n = \sum_{i=1}^{s} n_i$). Consider a polynomial kernel $k(x, x') = ((x, x'))^q$, with feature mapping $\phi(x) \in \mathcal{H} = \mathbb{R}^d$ such that $k(x, x') = \langle \phi(x), \phi(x') \rangle$. Let $\phi(A) \in \mathcal{H}^n$ denote the matrix obtained by applying $\phi$ on each column of $A$ and concatenating the resulting vectors. The goal of distributed KPCA is to find and send to each server a subspace of dimension $k$ that approximates $\phi(A)$. Thus it is also called (kernel) low rank approximation, and the subspace is called a low rank approximate subspace.

**Definition 1** A subspace $L \in \mathcal{H}^k$ is a rank-$k$ $(1 + \epsilon)$-approximate subspace for $\phi(A)$ if $L^\top L = I_k$ and

$$\|\phi(A) - LL^\top \phi(A)\|_F \leq (1 + \epsilon) \|\phi(A) - [\phi(A)]_k\|_F$$

where $[\phi(A)]_k$ is the best rank-$k$ approximation to $\phi(A)$.

Our main result is a randomized algorithm for distributed KPCA. It takes as input the local datasets, a rank $k$, and an error parameter $\epsilon$, and outputs a subspace that with constant probability is a relative-error approximation to the optimum. Roughly speaking, it first computes a set of weights measuring the importance of the data points for the task, and then samples according to the weights a small subset of points whose span are guaranteed to contain a good subspace. Finally, it computes such a good solution within the span of the sampled points. The three steps (weighting, sampling, and computing a solution) are all carefully designed by judiciously using (variants of) several techniques, to achieve the following bound on accuracy, communication and computation:

**Theorem 2** For polynomial kernels, there exists a randomized algorithm (Algorithm 1) that produces a subspace $L$ such that with probability at least 0.9, $L$ is a rank-$k$ $(1 + \epsilon)$-approximate subspace for $\phi(A)$. The total communication cost required is cost is $\tilde{O}(\frac{sdk}{\epsilon} + \frac{dk^2}{\epsilon^{1/3}})$.

The constant success probability can be boosted up to any high probability $1 - \delta$ by repetition, which adds only an extra $O(\log \frac{1}{\delta})$ term to the communication and computation. The output subspace $L$ is represented by $O(k/\epsilon)$ sampled points $Y$ from $A$ (i.e., $L = \phi(Y)C$ for some coefficient matrix $C \in \mathbb{R}^{|Y| \times k}$), so $L$ can be easily communicated and the projection of any data point on $L$ can be easily computed by the kernel trick. The communication cost has linear dependence on the dimension and the number of servers, and has no dependence on the number of data points (the $\tilde{O}$ only hides a factor of $\log k$). When $d > \frac{k}{\epsilon^2}$ and $k < e^{1/\epsilon}$.
which is typical for big data scenarios, the communication of our algorithm is $O(sdk/\epsilon)$, which matches the $O(sdk/\epsilon)$ cost of the state-of-the-art distributed linear PCA algorithm \cite{Balcan2014,Kannan2014}.

An immediate application is for distributed kernel $k$-means, which can be done by first computing KPCA to rank-$k/\epsilon$ and then $k$-means on the data projected on the subspace found by KPCA \cite{Dhillon2004,Dhillon2005}. Since there exist efficient distributed $k$-means algorithms \cite{Balcan2014}, our result leads to efficient algorithms for the polynomial kernel case.

**Corollary 3** Given a distributed $\alpha$-approximation $k$-means algorithm as a subroutine, there exists a randomized algorithm for polynomial kernels that with probability at least 0.9 produces a $(1+\epsilon)\alpha$-approximation solution for spectral clustering for $\phi(A)$. The total communication cost required is $O(sdk/\epsilon^2 + spoly(k/\epsilon))$ plus that of the subroutine on $O(k/\epsilon)$ dimensional data.

Our distributed KPCA algorithm amounts to sampling a small subset $Y$ from the original data set $A$ according to their importance such that the span of $\phi(Y)$ contains a good approximate subspace. The weights that measure their importance is statistical leverage scores, which play a key role in many modern randomized algorithms for linear algebra and matrix computation. Computing leverage scores needs to be done with care, as naive approaches lead to high communication and computational cost. We observe that for rank-$k$ approximation, it suffices to compute the generalized leverage scores with respect to rank $k$. So we can use the subspace embedding technique that summarizes the data and preserves the scores, and adopt a non-distributed fast algorithm for computing scores. Since computing leverage scores for linear or polynomial kernels in the distributed setting is a problem of independent interest, we summarize our result as follows. Note that leverage scores are typically used for sampling (e.g., in our algorithm), in which case constant approximation suffices and the communication is as low as $O(sk^2)$.

**Theorem 4** Suppose $\ell^{ij}$ is the statistical leverage score of the $j$-th column of $A^i$ in $A$ with respect to rank $k$ (see Definition 3). For polynomial kernels, there exists a randomized algorithm (Algorithm 4 in Section 3) that returns values $\tilde{\ell}^{ij}$, such that with probability at least 0.9, $|\ell^{ij} - \tilde{\ell}^{ij}| \leq \epsilon |\ell^{ij}|$ for all $i \in [s], j \in [n_i]$. The total communication cost required is $O(sk^2/\epsilon^4)$.

### 1.2 Overview of Main Techniques

As mentioned above, our algorithm consists of three steps: weighting points, sampling a subset, and computing a good solution from the subset. All the steps employ (variants of) randomized techniques in a careful way to achieve the desire bounds.

In the first step of computing leverage scores, our key technique is a subspace embedding, which projects the feature mapping of the data to a low dimension space while preserving the scores with respect to rank $k$, and thus allows for computing them with low communication depending on $k$ rather than on the dimension $d^i$. We use a communication efficient variant of the subspace embedding for polynomial kernels in \cite{Avron2014}: first perform their embedding, and then another embedding using i.i.d. Gaussian or fast Hadamard to further reduce the dimension. This way we can achieve both low communication and fast computation.

After computing leverage scores, one can simply sample according to them. However, it would give a $(1+\epsilon)$-approximation but with a rank-$O(k/\epsilon)$ space, not a rank-$k$ space. Fortunately, there exists an adaptive sampling approach that can start with and $O(1)$-approximation with rank $O(k)$ and produce $O(k/\epsilon)$ samples containing a rank-$k$ $(1+\epsilon)$-approximate subspace. So we first sample a subset of $O(k)$ points that achieves constant approximation, and then perform the adaptive sampling to pick $O(k/\epsilon)$ points $Y$ with the desired error bound.

The last step is then to find such a subspace within the span of $\phi(Y)$. Intuitively, one can just find the best rank-$k$ approximation for the projection of the data on the span of $\phi(Y)$. This naive approach has high cost depending on the number of points, but it can be improved by the following observation: it suffices to do so on a sketch of the projected data, which essentially reduces the number of points needed.

We review and provide the details of these building blocks needed for our algorithm in Section 2.
1.3 Related Work

There has been a surge of work on distributed machine learning, e.g., (Balcan et al., 2012; Zhang et al., 2012; Kannan et al., 2014; Balcan et al., 2014). The most related to ours are (Kannan et al., 2014; Balcan et al., 2014) which give efficient algorithms for linear PCA. Subspace embeddings are also the key element in the algorithm in the first paper. The second paper performs global PCA on top of local PCA solutions, but also uses subspace embeddings to obtain speedups. However, these algorithms cannot be directly adapted to the polynomial kernel case. The subspace embedding approach in (Kannan et al., 2014) will need to be performed on the explicit feature mapping, which is costly; the approach in (Balcan et al., 2014) requires sending the local PCA solutions, which need to be represented by the explicit feature mapping or by the set of all the local points, neither of which is practical. To the best of our knowledge, our algorithm is the first distributed kernel PCA algorithm with provable relative error and non-trivial bounds on communication and computation.

The key technique, that of a subspace embedding, has been extensively studied in recent years (Sarlós 2006; Achlioptas 2003; Arriaga and Vempala 1999; Ailon and Chazelle 2009; Clarkson and Woodruff 2013). The recent fast sparse subspace embeddings (Clarkson and Woodruff 2013) and its optimizations (Meng and Mahoney 2013; Nelson and Nguyen 2013) are particularly suitable for large scale sparse datasets, since their running time is linear in the number of non-zero entries in the data matrix. They also preserve the sparsity of the input data. The work of (Avron et al., 2014) shows that a fast computational approach, TENSORSKETCH, is indeed a subspace embedding for the polynomial kernel, which is a key tool used by our algorithm. Another element is leverage score sampling, which has a long history in data analysis for regression diagnostics and recently has been successfully used in the development of randomized matrix algorithms. See (Woodruff 2014) for a detailed discussion.

A prior work of Boutsidis et al. (Boutsidis et al., 2015) gives the first distributed protocol for column subset selection. Our work also selects columns, but our main advance over (Boutsidis et al., 2015) is that our protocol is the first to work for low rank approximation in the kernel space rather than the original space. Our result involves several key differences over (Boutsidis et al., 2015). For instance, the polynomial kernel can only be sketched on one side, so we first sketch that side, obtaining $S \cdot \phi(A)$, but then we can only hope to obtain leverage scores for $S \cdot \phi(A)$, which we do by a new distributed protocol. This turns out to be sufficient for us because we know $S \cdot \phi(A)$ contains a rank-$k O(1)$-approximation to $\phi(A)$ if $S$ has $\Theta(k)$ rows, and therefore if we sample $O(k \log k)$ columns of $\phi(A)$ proportional to the leverage scores of $S \cdot \phi(A)$ then the projection of $\phi(A)$ onto these columns has cost at most a constant factor times optimal. Another difference is that in all intermediate steps in our protocol we can only afford to communicate columns in the original space, that is, both the dimension $d^q$ and the number $n$ of examples are too large, whereas all prior protocols depend linearly on at least one of these quantities. This forces tasks such as adaptive sampling and computing an approximate subspace inside the columns found, that have been used in algorithms such as (Boutsidis and Woodruff 2014), to all be done implicitly, and we use the kernel trick several times to do so.

2 Review of Techniques

2.1 Notations

In the distributed setting, there are $s$ servers that are connected to a central processor. Server $i \in [s]$ has a local data set $A_i \in \mathbb{R}^{d \times n_i}$, and the global data set $A \in \mathbb{R}^{d \times n}$ is the concatenation of the local data $(n = \sum_{i=1}^{s} n_i)$.

For any matrix $M \in \mathbb{R}^{d \times n}$ and any $i \in [d], j \in [n]$, let $M_i$ denote the $i$-th row of $M$ and $M_j$ denote the $j$-th column of $M$. Let $\|M\|_F$ denote its Frobenius norm, and $\|M\|_2$ denote its spectral norm. Let $I_d$ denote the $d \times d$ identity matrix. Let the rank of $M \in \mathbb{R}^{d \times n}$ be $r \leq \min\{n, d\}$, and denote the SVD of $M$ as $M = USV^T$ where $U \in \mathbb{R}^{d \times r}, \Sigma \in \mathbb{R}^{r \times r}$, and $V \in \mathbb{R}^{n \times r}$.

For a kernel $k(x, x') = (x, x')^q$, let $\phi(\cdot) \in \mathcal{H}$ denote the corresponding feature mapping. Let $M \in \mathcal{H}$ denote a matrix in $\mathbb{R}^{d^q \times n}$ where each column is regarded as an element in $\mathcal{H}$ and let $\|M\|_{\mathcal{H}} = \text{tr}(M^TM)$. 4
For polynomial kernels, $\mathcal{H} = \mathbb{R}^d$ and $\langle \cdot , \cdot \rangle_\mathcal{H}$ is the regular dot product, and $\|M\|_\mathcal{H}$ is equivalent to $\|M\|_F$.

2.2 Subspace Embeddings

Subspace embeddings are a very useful technique that can improve the computational and space costs by embedding data points into lower dimension while preserving interesting properties needed. Formally,

**Definition 5** An $\epsilon$-subspace embedding of $M \in \mathbb{R}^{m \times n}$ is a matrix $S \in \mathbb{R}^{t \times m}$ such that for any vectors $x \in \mathbb{R}^n$,

$$\|SMx\|_2 = (1 \pm \epsilon) \|Mx\|_2.$$  

$Mx$ is in the column space of $M$ and $SMx$ is its embedding, so the definition means that the norm of any vector in the column space of $M$ is approximately preserved. Subspace embeddings can also be done on the right hand side, i.e., $S \in \mathbb{R}^{n \times t}$ and $\|x^\top MS\|_2 = (1 \pm \epsilon) \|x^\top M\|_2$ for any $x \in \mathbb{R}^m$. Our algorithm repeatedly makes use of subspace embeddings. In particular, the embedding we use is the concatenation of the following known subspace embeddings: COUNTSKETCH and i.i.d. Gaussians (or the concatenation of COUNTSKETCH, fast Hadamard and i.i.d. Gaussians). Due to space limitations, we do not present the details, which can be found in [Woodruff, 2014]; we only need the following fact.

**Lemma 6** For $M \in \mathbb{R}^{m \times n}$, there exist subspace embeddings $S \in \mathbb{R}^{t \times m}$ with $t = O(n/\epsilon^2)$. Furthermore, $SM$ can be successfully computed in time $O(mnz(M))$ with probability at least $1 - \delta$, where $nz(M)$ is the number of non-zero entries in $M$.

**Kernel subspace embeddings** Subspace embeddings can also be generalized for the feature mapping of kernels, simply by setting $M=\phi(A)$, $S \in \mathcal{H}^t$ and using the corresponding inner product in the definition. If the kernel subspace embedding suffices for solving the problem under consideration, then one only needs to deal with the data $S\phi(A)$ in much lower dimension rather than going to the feature mapping space. This is especially interesting for distributed kernel methods, since naively using the feature mapping or the kernel trick in this setting will leads to high communication cost. For our purpose, we will need the embedding matrix $S$ to have the following properties:

**P1** (Subspace Embedding): For any $V \in \mathcal{H}^k$ with orthonormal elements (that is, $V^\top V = I_k$), for all $x \in \mathbb{R}^k$, $\| (SV)x \|_2 = (1 \pm \epsilon_0) \| Vx \|_\mathcal{H}$, where $\epsilon_0$ is a sufficiently small constant.

**P2** (Approximate Product): For any $M \in \mathcal{H}^t$, $N \in \mathcal{H}^s$, $\| M^\top S^\top SN - M^\top N^\top \|_F \leq \sqrt{\epsilon} \| M \|_\mathcal{H} \| N \|_\mathcal{H}$.

The following lemma from [Avron et al., 2014] shows the implication of the two properties.

**Fact 1** Suppose $S$ satisfies $P1$ and $P2$, and suppose $E = S\phi(A)$ has SVD $E = USV^\top$. Then we have

$$\| [\phi(A)V]_k V^\top - \phi(A) \|_\mathcal{H} \leq (1 + \epsilon) \| \phi(A) - [\phi(A)V]_k \|_\mathcal{H}.$$  

Since $\phi(A)V$ is the projection of $\phi(A)$ onto the row space of $S\phi(A)$ and $[\phi(A)V]_k$ is the best rank-$k$ approximation there, Lemma 1 means that the row space of $S\phi(A)$ contains a good approximation to $\phi(A)$, up to rank-$k$ approximation error. As discussed below, $E$ can be used to compute the generalized leverage for $\phi(A)$, which then suffices for rank-$k$ approximation.

For polynomial kernels, there exists an efficient algorithm TENSORSKETCH to compute the embedding. However, the embedding dimension has a quadratic dependence on the rank $k$, which will increase the communication. Fortunately, as inLemma 6 subspace embedding can be concatenated, so we can further apply another known subspace embedding such as i.i.d. Gaussians or fast Hadamard which, though not fast for feature mapping, is fast for the already embedded data and has lower dimension. In this way, we can enjoy the benefits of both approaches.
Lemma 7 For the polynomial kernel $k(x, x') = \langle x, x' \rangle^d$, there exists a subspace embedding matrix $S \in \mathbb{R}^{t \times d^s}$ that satisfies $P1$ and $P2$ with $t = O(k/\epsilon)$. Furthermore, such $S\hat{\phi}(A)$ can be successfully computed with probability at least $1 - \delta$ in time $\tilde{O} \left( \left( \frac{k}{\epsilon^2} + q \right) \text{nnz}(A) + \frac{q \text{nnz}(A)}{\epsilon^S} \right)$.

Proof First use TensorSketch (Avron et al., 2014) to bring the dimension down to $O(3^d k^2 + k/\epsilon)$. Then, we can use an i.i.d. Gaussian matrix, which reduces it to $t = O(k/\epsilon)$; or we can first use fast Hadamard transformation to bring it down to $O(\text{polylog}(k)/\epsilon)$, then multiply again by i.i.d Gaussians to bring down to $O(k/\epsilon)$.

$P1$ follows immediately from the definition, so we only need to check the matrix product. Let $S = \Omega T$ where $T$ is the TensorSketch matrix and $\Omega$ is an i.i.d. Gaussian matrix. Since they are both subspace embedding matrices, then for any $M$ and $N$,

$$\|M^\top S^\top SN - M^\top T^\top TN\|_F \leq \sqrt{\frac{\epsilon}{k}} \|MT\|_F \|NT\|_F,$$

$$\|M^\top T^\top TTN - M^\top TN\|_F \leq \sqrt{\frac{\epsilon}{k}} \|M\|_H \|N\|_H.$$

By the subspace embedding property, $\|MT\|_F = (1 \pm \epsilon_0) \|M\|_H$ and $\|NT\|_F = (1 \pm \epsilon_0) \|N\|_H$ for some small constant $\epsilon_0$. Combining all these bounds and choosing proper $\epsilon$, we know that $S = \Omega T$ satisfies $P2$. $\blacksquare$

2.3 Leverage Score Sampling

The statistical leverage scores measure the nonuniform structure that is critical for importance sampling in fast randomized algorithms for many problems; see (Mahoney, 2011) for more discussion. Sampling according to leverage scores fits distributed Kernel PCA, since it leads to small sample size while providing a good approximation of the original data. In fact, for our purpose, it suffices to consider a generalized notion of leverage scores with respect to rank $k$. To provide more details, we begin with the definition.

Definition 8 For $E \in \mathbb{R}^{t \times n}$ with SVD $E = U\Sigma V^\top$, the leverage score $\ell_i$ for its $i$-th column is the squared $\ell_2$ norm of the $i$-th column of $V^\top$. Formally, $\ell_i = \|V_{i1}\|_2^2$.

If $E$ can approximate the row space of $M$ up to $\epsilon$, i.e., $\|XE - M\|_F \leq (1 + \epsilon) \|M - [M]_k\|_F$, then $\{\ell_i\}$ are also called the leverage scores for $M$ with respect to rank $k$.

A key property of leverage scores is that a small set of columns sampled according to the leverage scores will span a subspace that is close to the subspace spanned by all the columns, e.g., Theorem 5 in (Drineas et al., 2008):

Fact 2 Suppose $E \in \mathbb{R}^{t \times n}$ has rank at most $r$, $M \in \mathbb{R}^{m \times n}$ and $\epsilon \in (0, 1]$. Let $\ell_i$ be the leverage scores of the $i$-th column in $E$. Define sampling probabilities $p_i$ such that for some $\beta \in (0, 1)$, $p_i \geq \frac{\beta \ell_i}{\sum_{j=1}^n \ell_j}$, for all $i \in [n]$. Sample $M^{(i)}$ with probability $\min \left\{1, O(\frac{\log r}{\epsilon \beta})p_i \right\}$. Define an $n \times n$ diagonal sampling matrix $T$ for which $T_{i,i} = 1/\sqrt{\ell_i}$ if $M^{(i)}$ is sampled, and $T_{i,i} = 0$ otherwise. Then with probability at least $.9$,

$$\|M - MT(ET)^\dagger E\|_F \leq (1 + \epsilon) \min_X \|M - XE\|_F.$$

Note that the theorem is stated in the general form: the leverage scores of the columns of $E$ are used for sampling the columns of $M$. A special case is when the rowspace of $E$ approximates the row space of $M$, i.e., there exists $X$ such that $\|M - XE\|_F$ is small. In this case, the sampling error is guaranteed to be small, and at the same time $\ell_i$ are just the leverage scores for $M$ with respect to rank $k$ by Definition 8. Therefore, Fact 2 means sampling columns of $M$ according to its generalized scores leads to small error for

\footnote{This generalizes the definition in (Drineas et al., 2012) by allowing $E$ to have rank larger than $k$.}
data to its projection on approximate subspace. Then adaptive sampling \( \alpha \) that the scores are used for later sampling, and a square of the distance from \( \phi \). Fact 3 Suppose the span of \( M \) holds.

2.4 Adaptive Sampling

Leverage score sampling for \( M = \phi(A) \) contains a rank-\( O(k/\epsilon) \) \((1 + \epsilon)\)-approximation to \( \phi(A) \). This is still not the desired guarantee. Therefore, we first sample a constant approximation and then resort to the adaptive sampling algorithm in (Deshpande and Vempala, 2006; Boutsidis and Woodruff, 2014), which can reduce the bound to a linear dependence. The algorithm computes the errors of the points to the constant approximation and then samples accordingly \( O(k/\epsilon) \) points whose span is guaranteed to contain a \((1 + \epsilon)\)-approximation. Formally,

\[
\text{Fact 3} \quad \text{Suppose the span of } \phi(P) \text{ contains a constant rank-} k \text{ approximation for } \phi(A), \text{ and let } r^i \text{ to be the square of the distance from } \phi(A, i) \text{ to its projection on the subspace spanned by } \phi(P). \text{ Sample a set of } O(k/\epsilon) \text{ points } Y \text{ from } A \text{ according to } r^i. \text{ Then the span of } \phi(Y) \text{ contains a } (1 + \epsilon) \text{-approximation for } \phi(A).
\]

3 Algorithm

The distributed kernel PCA algorithm, described in Algorithm 1, consists of three steps. First, the algorithm computes a constant approximation of the generalized leverage scores for \( \phi(A) \) with respect to rank \( k \). Note that the scores are used for later sampling, and a \( \alpha \)-approximation leads to an extra term \( O(\alpha) \) in the sample size, so a constant approximation is sufficient. Algorithm 2 describes how to compute an \( \alpha \)-approximation. Since we only need the generalized scores w.r.t. rank \( k \), so we can do subspace embedding to dimension \( t = O(k/\alpha) \), and then compute the scores of the embedded data \( E = [E^1, \ldots, E^s] \). Again, we only need to approximate the scores of \( E \), so we can apply another embedding to reduce the number of data points. Let \( ET = [E^1T^1, \ldots, E^sT^s] \) denote the embedded data, and do QR factorization \((ET)^\top = UZ\). Now, the rows of \( U^\top = (Z^\top)^{-1}ET \) are a set of basis for \( ET \). Then, think of \( U^\top T^1 = (Z^\top)^{-1}E \) are the basis for \( E \), so we can simply compute the norm of the columns in \((Z^\top)^{-1}E\).

In the second step, the algorithm samples a subset of points \( Y \) that acts as a proxy for the original data. We first sample a set \( P \) of \( O(k \log k) \) points according to the scores, which then contains a constant approximate subspace. Then adaptive sampling \( O(k/\epsilon) \) points according to the square distance from the data to its projection on \( P \) leads to the desire \( Y \).
\section{Analysis}

\subsection{Approximate Leverage Scores: Proof of Theorem 4}

First, by Fact 4, we know that the row space of the embedding matrix $E = S\phi(A)$ contains enough information about the range of $\phi(A)$. Then the scores for $E$ are the generalized scores for $\phi(A)$. Note that Algorithm 2 can be viewed as applying an embedding $T = \text{diag}(T^1, \ldots, T^s)$ on $E$ to approximate the scores while saving the costs. Such a scheme has been analyze in Drineas et al. 2012. Let $\ell^j$ be the leverage score of $(E^i)_{ij}$ in $E$. Then the analysis in Drineas et al. 2012 essentially leads to:

**Fact 4** If $T$ is an $\epsilon_0$-subspace embedding, then we have $\tilde{\ell}^j = (1 \pm \epsilon_0)\ell^j$. 

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**Algorithm 2** Distributed Leverage Score disLS

**Input:** $\{A^i\}_{i=1}^s$, rank $k$, $\epsilon$

**Output:** $(1 + \epsilon)$-approx leverage $\tilde{\ell}^j$ w.r.t. rank $k$

1: Each server $i$:
   - embed $E^i = S\phi(A^i) \in \mathbb{R}^{t \times w}$, $t = O(k/\epsilon)$;
   - embed $E^i T^i \in \mathbb{R}^{t \times p}$, $p = O(t/\epsilon^2)$.
2: Center: QR-factorize $[E^1 T^1, \ldots, E^s T^s]^\top = UZ$.
3: Each server $i$: compute $\tilde{\ell}^j = \|((Z^\top)^{-1} E^i)_{ij}\|_2^2$.

**Algorithm 3** Distributed Low Rank disLR

**Input:** $\{A^i\}_{i=1}^s$, subset $Y$, rank $k$

**Output:** rank-$k$ subspace $L = QW$

1: Each server $i$:
   - compute the basis $Q$ for $\phi(Y)$;
   - compute the projection $\Pi_i = Q^\top \phi(A^i)$;
   - embed $\Pi_i T_i \in \mathbb{R}^{Y \times w}$, $w = O(|Y|/\epsilon^2)$.
2: Center:
   - concatenate $\Pi IT = [\Pi^1 T^1, \ldots, \Pi^s T^s]$;
   - compute the top $k$ singular vectors $W$ of $\Pi IT$.

Finally, the algorithm computes a subspace $L$ from the span of $\phi(Y)$. We first project the data on the span to get the low dimension data $\Pi$. Now it suffices to compute the best rank-$k$ approximation for $\Pi$. Again, since we only need approximation, we can do an embedding to reduce the number of data points and get $\Pi IT = [\Pi^1 T^1, \ldots, \Pi^s T^s]$. Then we compute the best rank-$k$ approximation $W$ for $\Pi IT$, which is then a good approximation for $\Pi$ and thus $\phi(A)$. The algorithm then returns $L$, the representation of $W$ in the coordinate system of $\phi(A)$.

A few details need to be specified. In computing the final solution from $Y$, we need to compute the projection of $\phi(A)$ onto $\phi(Y)$. This can be done by using kernel trick and implicit Gram-Schmidt. Note that $\Pi^i = Q^\top \phi(A^i)$ where $Q$ is the basis for $\phi(P)$. Suppose $\phi(Y)$ has QR-factorization $\phi(Y) = QR$. Then $Q = \phi(Y) R^{-1}$ and $Q^\top \phi(A) = (R^{-1})^\top \phi(Y)^\top \phi(A)$ where $\phi(Y)^\top \phi(A)$ is just the kernel value between points in $Y$ and points in $A$. For $R$, we have $Q^\top Q = (R^{-1})^\top \phi(Y)^\top \phi(Y) R^{-1} = I$, so $R^\top R = \phi(Y)^\top \phi(Y)$ and thus $R$ can be computed by factorizing the kernel matrix on $Y$.

Similarly, to compute the distance for adaptive sampling, we first need to compute the projection of $\phi(A)$ onto $\phi(P)$, which can be done in the same way. Then the square distance from the original data to the projection can be computed by subtracting the square norm of the projection from the square norm of the original data.
It now suffices to show that $T$ is an $O(\epsilon)$-subspace embedding. When $p = O(t/\epsilon)$, each $T^i$ is an $O(\epsilon)$-subspace embedding matrix, and thus by simple calculation $T$ is $O(\epsilon)$-subspace embedding. Then we approximate the leverage scores up to a factor of $\epsilon$.

### 4.2 Leverage Score Sampling

Now, we are ready to show the following key lemma.

**Lemma 9** In Algorithm 2, the span of $\phi(Y)$ contains a $(1 + \epsilon)$-approximation rank-$k$ subspace for $\phi(A)$.

**Proof** By Fact 3, it suffices to prove that the span of $\phi(P)$ contains a constant approximation. Suppose $E$ has SVD $E = U\Sigma V^T$. By Fact 4, $\tilde{\ell}^{ij} \in [1/2, 3/2]\ell^{ij}$ where $\ell^{ij}$ is the true leverage score for the column $E^j_i$ in $E$. Then sampling according to $\tilde{\ell}^{ij}$ means the sampling probabilities satisfy the condition in Fact 2 with some constant $\beta$, so

$$\|\phi(A) - \phi(A)T(ET)^\dagger E\|_\mathcal{H} \leq O(1) \min_{X \in \mathcal{H}} \|\phi(A) - XE\|_\mathcal{H}.$$ 

Now let $X = [V\phi(A)]_k \Sigma^{-1} U^T$, so that

$$\|XE - \phi(A)\|_\mathcal{H} = \|[\phi(A)V]_k V^T - \phi(A)\|_\mathcal{H} \leq O(1) \|\phi(A) - [\phi(A)]_k\|_\mathcal{H},$$

where the last step follows from Fact 1 and our choice of $t$. This leads to

$$\|\phi(A) - \phi(A)T(ET)^\dagger E\|_\mathcal{H} \leq O(1) \|\phi(A) - [\phi(A)]_k\|_\mathcal{H}.$$ 

Note that $T$ is the sample matrix to get $P$ from $A$, so $\phi(A)T$ can be written as $\phi(P)T'$ for some $T'$. Then $C = T'(ET)^\dagger E$ satisfies

$$\|\phi(A) - \phi(P)C\|_\mathcal{H} \leq O(1) \|\phi(A) - [\phi(A)]_k\|_\mathcal{H}$$

which completes the proof.

### 4.3 Compute Approximate Subspace

**Lemma 10** In Algorithm 3, if the span of $\phi(Y)$ contains a $(1 + \epsilon)$-approximate subspace, then

$$\|LL^T \phi(A) - \phi(A)\|_\mathcal{H} \leq (1 + \epsilon)^2 \|\phi(A) - [\phi(A)]_k\|_\mathcal{H}.$$ 

**Proof** For our choice of $w$, $T^i$ is an $\epsilon$-subspace embedding matrix for $\Pi_i$. Then their concatenation $B$ is an $\epsilon$-subspace embedding for $\Pi$, the concatenation of $\Pi_i$. This can be shown by the similar argument as in Fact 4. Then we can apply the argument in Lemma 5 in (Avron et al., 2014) (also implicit in Theorem 1.5 in (Kannan et al., 2014)).

Now our main result Theorem 2 just follows by combining Lemma 9, Fact 3 and Lemma 10.

### 5 Experiments

We demonstrate the effectiveness of our algorithm in three tasks: 1) Kernel PCA, 2) Kernel PCA then distributed $k$-means clustering, and 3) Kernel PCA then regression. Since there is no existing distributed kernel PCA algorithm to the best of our knowledge, and since the key of our algorithm is to adaptively select
a small subset of meaningful points, we compare with the baseline that uniformly samples data from the dataset and then performs Algorithm 8 to extract kernel principle components. For regression, in addition to uniform sampling, we also compare with another baseline (called sketching-PCA) that first applies tensor-sketch to reduce the data into a lower-dimensional space, then performs distributed PCA (not kernel PCA), and finally runs linear regression on the top principle components.

Methodology The data is partitioned on different nodes according to power law distribution with exponent 2. Depending on the size of the dataset, the number of nodes used ranges from 5 to 200. We run the algorithms under the same communication budget and compare their errors. The evaluation criteria are the low rank approximation error for distributed KPCA task, and the $k$-means cost for the clustering task. For regression, we compare the normalized $\ell_2$ error: suppose the ground truth target is $y$, and the prediction is $y_p$, we report $\|y - y_p\|/\|y\|$. Each algorithm is run 5 times; the mean and the standard deviation are then plotted.

Datasets We use: 1) 20 newsgroup (61118 points of dimension 11269); 2) CT-slice (384 $\times$ 53500); 3) Year-Prediction MSD (90 $\times$ 463715); 4) MNIST8M (784 $\times$ 8000000); 5) HIGGS (28 $\times$ 11000000); 6) SUSY (18 $\times$ 3000000); 7) BoW PubMed (141043 $\times$ 8200000); 8) Protein Structure (9 $\times$ 45730). Distributed KPCA and clustering are carried out on 1)-7), and regression is carried out on 2), 3) and 8). Most datasets are from UCI Repository [Bache and Lichman 2013; Baldi et al. 2014].

Results Figure 1 shows the low rank approximation error in the distributed kernel PCA task. It can be observed that using the same amount of communication, our algorithm outperforms the baseline. Uniform sampling uses about 5 times more communication to achieve a certain small error, or simply cannot achieve the same error as our algorithm does. Figures 2 shows the running time of the algorithms. The time of our algorithm is about twice that of uniformly sampling. The additional time spent is on approximating leverage scores and calculating the residues for adaptively sampling. With additional computational costs, our algorithm is able to achieve smaller errors given the same communication budget. Note that, in practice, communication overhead is usually much larger than computational time. Therefore, the additional computation effort is justified for reducing the communication overhead. Also note that uniform sampling is basically reducing big data to small data. If the problem at hand only requires small data (e.g., the leverage scores are quite uniform) or if one is satisfied with moderate performance that can be achieved by small data (obtained by uniform sampling), then uniform sampling should be used. But if one wants to take advantage of big data, then our approach is better, which can handle much larger data using only twice computation cost and similar or even less communication.
Figure 2: KPCA run-time vs communication

Figure 3: KPCA + distributed k-means (sum of squared costs)

Figure 4: KPCA + distributed k-means run-time vs communication
Figure 5: KPCA + regression

Figure 6: KPCA + regression run-time vs communication

Figure 3 shows the error in the $k$-means clustering task and Figure 4 shows the running time. Similar results are observed as in the distributed kernel PCA task. For example, on HIGGS the error of uniform sampling is almost twice that of ours, while the running time is almost the same.

Figures 5 shows the error in the regression task and Figure 6 shows the running time. In this task, we vary the number of principle components extracted for linear regression and compare the normalized regression error. We can see the sketching-PCA method incurs higher errors in all datasets, and requires more time in some datasets. Uniformly sampling and our method have similar performance in the regression task. It is likely that the top few principle components do not contain enough relevant information for the target variables. In addition, our theoretical bound is on the low-rank approximation error and it may not be linearly correlated with regression error.

Finally, in Figure 7 we plot the leverage scores of the datasets. We can see that some datasets, such as MNIST8M and CT-Slice, have more uniform leverage scores than other datasets, such as 20 newsgroup and HIGGS. Compared with the performance result, we can see that the uniformity of the leverage scores is correlated with the performance gap between our algorithm and uniform sampling. For large datasets with non-uniform leverage scores, our proposed algorithm has more significant advantages over the baseline.

6 Conclusion

This paper proposes a distributed algorithm for Kernel Principal Component Analysis, and provides theoretical bounds and empirical support for the polynomial kernel case. In this case, the algorithm computes a relative-error approximation compared to the best rank-$k$ subspace, using communication that nearly matches that of the state-of-the-art algorithms for distributed linear PCA. This is the first distributed algorithm that can achieve such provable approximation and communication bounds. The experimental results show that our algorithm can achieve better performance than the baseline using the same communication budget.
Figure 7: Leverage scores for each dataset

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