Scale Up Nonlinear Component Analysis with Doubly Stochastic Gradients

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Abstract

Nonlinear component analysis such as kernel Principle Component Analysis (KPCA) and kernel Canonical Correlation Analysis (KCCA) are widely used in machine learning, statistics and data analysis, and they serve as invaluable preprocessing tools for various purposes such as data exploration, dimension reduction and feature extraction.

However, existing algorithms for nonlinear component analysis cannot scale up to millions of data points due to prohibitive computation and memory requirements. There are some recent attempts to scale up kernel version of component analysis using random feature approximations. However, to obtain high quality solutions, the number of required random features can be the same order of magnitude as the number of data points, making such approach not directly applicable to the regime with millions of data points.

We propose a simple, computationally efficient, and memory friendly algorithm based on the “doubly stochastic gradients” to scale up a range of kernel nonlinear component analysis, such as kernel PCA, CCA, SVD and latent variable model estimation. Despite the non-convex nature of these problems, we are able to provide theoretical guarantees that the algorithm converges at the rate $\tilde{O}(1/t)$ to the global optimum, even for the top $k$ eigen subspace. We demonstrate the effectiveness and scalability of our algorithm on large scale synthetic and real world datasets.

1 Introduction

Component analysis, especially Principal Component Analysis (PCA) and Correlation Component Analysis (CCA), are basic and popular techniques in statistics, machine learning, and data analysis. They can discover important features and patterns in unlabeled datasets, and thus have many applications, such as exploration, visualization, approximation and denoising of the data. The importance of component analysis become even more significant in the era of big data, since the extraction of components allows downstream applications such as classification and regression to exploit useful information in large datasets in a computationally efficient way.

Most, if not all, large scale datasets have inherent nonlinear structures, which leads to increasing interests in kernel component analysis, such as kernel PCA [28], kernel SVD [8], kernel CCA [1], and kernel ICA [5]. These methods extend component analysis to data mapped to the kernel feature space. Since the vectors in the kernel feature space correspond to nonlinear functions in the original space, they enable the exploitation of the nonlinear structure, allowing one to do nonlinear dimension reduction or discover nonlinear latent components. This is crucial for complex data such as text and images, which are abundant nowadays.

However, the applicability of kernel component analysis on large-scale datasets has been limited due to prohibitive computation and memory requirement. Recently, methods such as Randomized Component Analysis [19] are able to scale to larger datasets by leveraging random feature approximation. Such methods approximate the kernel function by using explicit random feature mappings. Subsequent component analysis

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steps can thus be performed in the primal form, resulting in usually linear computational complexity. Moreover, the dimension of the random features used is much smaller than the explicit feature dimension and the number of data point, to avoid prohibitive computation. However, theoretical analysis [24, 19] shows that in order to get high quality results, the number of random features should grow linearly with the number of data points. Experimentally, one often sees that the statistical performance of the algorithm usually improves as one increases the number of random features.

Another approach to scale up the kernel component analysis is to use stochastic gradient descent and online updates. There are an abundance of literature on online component analysis, notably among which are Oja’s update rules [20, 21]. These stochastic update methods have also been extended to the kernel case [17, 9, 15]. They require much less computation than their batch counterpart, converge in $O(1/t)$ rate, and are naturally applicable to streaming data setting. However, they share a severe drawback: all data points used in the updates need to be kept for testing, rendering them impractical for large datasets.

In this paper, we propose to use the “doubly stochastic gradients” for nonlinear component analysis. This technique is a general framework for scaling up kernel methods [11] for convex problems and has been successfully applied to many popular kernel machines such as kernel SVM, kernel ridge regressions, and Gaussian process. It uses two types of stochastic approximation simultaneously: random data point instead of the whole dataset (as in stochastic update rules), and random features instead of the true kernel functions (as in randomized component analysis). These two approximations lead to several benefits.

- **Computation efficiency** The key computation in each step is the generation of a mini-batch of random features and the evaluation of these features on a mini-batch of data points, which can be done efficiently.

- **Memory efficiency** The training data points need not be stored, as we can just keep a small program for regenerating the random features, and sample previously used random features according to pre-specified random seeds. The regeneration of the random features results in a small overhead of time which is negligible compared to the existing computation, but leads to huge saving in memory: the memory requirement up to step $t$ is $O(t)$, independent of the dimension of the data.

- **Adaptibility** The doubly stochastic gradient approach can adaptively grow the number of random features, which is particularly suitable for streaming data. Unlike the previous approaches that can only work with a fixed number of random features beforehand, our approach is able to increase the model complexity by using more features when new data points arrive, and thus enjoys the advantage of nonparametric methods.

Therefore, this framework is preferable for kernel methods on large datasets. However, it is a prior unclear how to apply it to non-convex problems common in component analysis, and whether the solution will converge to the global optimum, and if so, how fast the convergence rate is. In this paper, we address these questions and make the following contributions.

- **General framework for kernel component analysis** We show that the general framework of doubly stochastic updates can be applied in various kernel component analysis tasks, including kernel PCA, kernel SVD, kernel CCA, etc.. Since kernel PCA is a key and typical component analysis task, we focus on it in the paper and provide a description of other tasks in Section 6. Although we only state the guarantee for kernel PCA, the analysis can also be extended to the other tasks.

- **Strong theoretical guarantee** We focus on kernel PCA and prove that the finite time convergence rate of doubly stochastic approach is $\hat{O}(1/t)$. We note that [11] has provided similar guarantees for using doubly stochastic approaches to solve problems such as kernel SVM and ridge regression. However, the setting in this paper is quite different from that in [11], which crucially relied on the convexity of the optimization problem. In contrast, in this paper the optimization objective is not convex (in fact, it is concave everywhere). We also note that the existing analysis for stochastic updates crucially relies on the fact that the computed eigenfunctions are in the kernel feature space, while in our case they
can be out of the feature space due to the random feature approximation. Therefore, our analysis are quite different from these existing analysis.

- **Strong empirical performance** The convergence rate, together with the efficient computation and memory consumption, allows the doubly stochastic approach to scale up to datasets consisting of millions of data points. Also, as a result of being able to use many more random features, the algorithm can often find much better solutions than methods that can only use a limited number of random features. We demonstrate such benefits on both synthetic and real world datasets.

2 Related work

Kernel PCA was first proposed in [29] and has been a standard tool for extracting the nonlinear structure of data. However, naive approaches are not scalable due to prohibitive computation and memory requirement. Random feature approach [23, 24], which approximates the kernel function using explicit random feature mappings, is a popular technique that can alleviate the difficulty. It has been applied to various kernel methods [18, 11, 19], among which most related to our work is Randomized Component Analysis [19]. One drawback of Randomized Component Analysis is that their theoretical guarantees are only for kernel matrix approximation. It does not say anything about the solution obtained from randomized PCA is close to the true solution. In contrast, we provide a finite time convergence rate of how our solution approaches the true solution. In addition, a moderate size of random features can work well for tens of thousands of data points, but datasets with tens of millions of data points require much more random features. Our online approach allows the number of random features, hence the flexibility of the function class, to grow with the number of data points. This makes our method suitable for data streaming setting, which is not possible for previous random feature approaches.

Online algorithms for PCA have a long history. Oja proposed two stochastic update rules for approximating the first eigenvector and provided convergence proof in [20, 21], respectively. These rules have been extended to the generalized Hebbian update rules [26, 31, 6] that compute the top \(k\) eigenvectors (the subspace case). Similar ones have also been derived from the perspective of optimization and stochastic gradient descent [31, 3]. They are further generalized to the kernel case [17, 9, 15]. However, online kernel PCA needs to store all the training data points for testing, which is impractical for large datasets. Our doubly stochastic method avoids this problem by using random features and keeping only a small program for regenerating previously used random features according to pre-specified seeds, thus it can scale up to tens of millions of data points.

For finite time convergence rate, [6] provided an analysis for computing the first eigenvector in linear PCA using Oja’s rule. A new stochastic update rule for the same purpose is proposed in [32] and its convergence rate is analyzed. [14] provided an analysis for the subspace case using noisy power method which requires explicit normalization, which is infeasible for kernel PCA. We provide finite time convergence rates for the subspace case using stochastic and doubly stochastic updates, which hold for both with and without normalization.

Besides kernel PCA, there are other kernel component analysis, such as kernel SVD [8], kernel CCA [11], and kernel Fisher discriminant analysis [30]. These problems are closely related, and the techniques for one can typically be applied to the others. Therefore, we focus on kernel PCA and provide the extensions of our approach to these tasks in Section 6.
3 Preliminaries

3.1 Kernels and Covariance Operators

A kernel \( k(x, y) : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R} \) is a function that is positive-definite (PD), i.e., for all \( n > 1, c_1, \ldots, c_n \in \mathbb{R} \), and \( x_1, \ldots, x_n \in \mathcal{X} \), we have
\[
\sum_{i,j=1}^{n} c_i c_j k(x_i, x_j) \geq 0.
\]

A reproducing kernel Hilbert space (RKHS) \( \mathcal{F} \) on \( \mathcal{X} \) is a Hilbert space of functions from \( \mathcal{X} \) to \( \mathbb{R} \). \( \mathcal{F} \) is an RKHS if and only if there exists a \( k(x, x') : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R} \) such that \( \forall x \in \mathcal{X}, k(x, \cdot) \in \mathcal{F} \), and \( \forall f \in \mathcal{F}, \langle f(\cdot), k(x, \cdot) \rangle_{\mathcal{F}} = f(x) \). If such a \( k(x, x') \) exist, it is unique and it is a PD kernel. A function \( f \in \mathcal{F} \) if and only if \( \| f \|^2_{\mathcal{F}} := \langle f, f \rangle_{\mathcal{F}} < \infty \).

Given a distribution \( P(x) \), a kernel function \( k(x, x') \) with RKHS \( \mathcal{F} \), the covariance operator \( A : \mathcal{F} \mapsto \mathcal{F} \) is a linear self-adjoint operator defined as
\[
Af(\cdot) := \mathbb{E}_x[f(x) k(x, \cdot)], \quad \forall f \in \mathcal{F},
\]
and furthermore
\[
\langle g, Af \rangle_{\mathcal{F}} = \mathbb{E}_x[f(x) g(x)], \quad \forall g \in \mathcal{F}.
\]

Let \( F = (f_1(\cdot), f_2(\cdot), \ldots, f_k(\cdot)) \) be a list of \( k \) functions in the RKHS, and we define matrix-like notation
\[
AF(\cdot) := (Af_1(\cdot), \ldots, Af_k(\cdot)),
\]
and \( F^\top AF \) is a \( k \times k \) matrix, whose \( (i, j) \)-th element is \( \langle f_i, Af_j \rangle_{\mathcal{F}} \). The outer-product of a function \( v \in \mathcal{F} \) defines a linear operator \( vv^\top : \mathcal{F} \mapsto \mathcal{F} \) such that
\[
(vv^\top)f(\cdot) := \langle v, f \rangle_{\mathcal{F}} v(\cdot), \quad \forall f \in \mathcal{F}
\]
Let \( V = (v_1(\cdot), \ldots, v_k(\cdot)) \) be a list of \( k \) functions, then the weighted sum of a set of linear operators, \( \{v_i v_i^\top\}_{i=1}^k \), can be denoted using matrix-like notation as
\[
V\Sigma_k V^\top := \sum_{i=1}^k \lambda_i v_i v_i^\top
\]
where \( \Sigma_k \) is a diagonal matrix with \( \lambda_i \) on the \( i \)-th entry of the diagonal.

3.2 Kernel PCA

Kernel PCA aims to identify the top \( k \) eigenfunctions \( V = (v_1(\cdot), \ldots, v_k(\cdot)) \) for the covariance operator \( A \), where \( V \) is also called the top \( k \) subspace for \( A \).

A function \( v \) is an eigenfunction of covariance operator \( A \) with the corresponding eigenvalue \( \lambda \) if
\[
Av(\cdot) = \lambda v(\cdot).
\]
Given a set of eigenfunctions \( \{v_i\} \) and associated eigenvalues \( \{\lambda_i\} \), where \( \langle v_i, v_j \rangle_{\mathcal{F}} = \delta_{ij} \). We can denote the eigenvalue of \( A \) as
\[
A = V\Sigma_k V^\top + V_\perp \Sigma_\perp V_\perp^\top
\]
Table 1: Example of kernels and their random feature representation

| Kernel          | $k(x, x')$                              | $\phi_k(x)$                        | $p(\omega)$                                                                 |
|-----------------|-----------------------------------------|------------------------------------|-------------------------------------------------------------------------------|
| Gaussian [23]   | $\exp(-\|x-x'\|^2_2)$                  | $\exp(-i\omega^\top x)$           | $2\pi^{-\frac{d}{2}}\exp(-\|\omega\|^2_2)$                                |
| Laplacian [24]  | $\exp(-\|x-x'\|_1)$                    | $\exp(-i\omega^\top x)$           | $\prod_{i=1}^d \frac{1}{\pi(1+i\omega^2)}$                                 |
| Cauchy [23]     | $\prod_{i=1}^d \frac{1}{1+(x_i-x'_i)^2}$ | $\exp(-i\omega^\top x)$           | $\exp(-\|\omega\|_1)$                                                      |
| Matérn [25]     | $\frac{2^{1-v}}{\Gamma(v)} \left(\frac{\sqrt{2v}\|x-x'\|_2}{\ell}\right)^v K_v \left(\frac{\sqrt{2v}\|x-x'\|_2}{\ell}\right)$ | $\exp(-i\omega^\top x)$           | $\frac{\pi^\nu 4^\nu \|\omega\|^2_2}{\Gamma(\nu+\frac{d}{2})\Gamma(\nu+1)} \left(\frac{2\pi^2 + 4\pi^2 \|\omega\|^2_2}{\nu+\frac{d}{2}}\right)^{\nu+\frac{d}{2}}$ |
| Dot Product [16]| $\sum_{n=0}^\infty a_n (x,x')^n \quad a_n \geq 0$ | $\sqrt{\alpha} N^{p+1} \prod_{i=1}^N \omega_i^x x$ | $\mathbb{P}[N=n] = \frac{1}{n^{p+1}}$                                    |
| Polynomial [22] | $\exp(-\beta \sum_{i=1}^d \sqrt{x_i + x'_i})$ | $\exp(-i\omega^\top x)$           | $C_j = S_j D_j$, $D_j \in \mathbb{R}^{d \times d}$, $S_j \in \mathbb{R}^{D \times d}$ |
| Exp-Semigroup [36]| $\prod_{i=1}^d \frac{x_i + x'_i}{x_i + x'_i + \lambda}$ | $\exp(-i\omega^\top x)$           | $\prod_{i=1}^d \frac{1}{\sqrt{2\pi}} \omega_i \exp\left(-\frac{\omega_i}{2\omega_i^2}\right)$ |
| Rec-Semigroup [36]| $\prod_{i=1}^d \frac{x_i + x'_i}{x_i + x'_i + \lambda}$ | $\exp(-i\omega^\top x)$           | $\prod_{i=1}^d \lambda \exp(-\frac{\omega_i}{2\omega_i^2})$                |
| Arc-Cosine [10] | $\frac{1}{\sqrt{2}} \|x\|^n \|x'\|^n J_n(\theta)$ | $\exp(-i\omega^\top x)$           | $2\pi^{-\frac{d}{2}} \exp(-\|\omega\|^2_2)$                                |

$D_j$ is random $\{\pm 1\}$ diagonal matrix and the columns of $S_j$ are uniformly selected from $\{e_1, \ldots, e_D\}$. $\nu$ and $\ell$ are positive parameters. $K_v$ is a modified Bessel function. $\odot$ stands for element-wise product. $\theta = \cos^{-1} \frac{x_i x'_i}{\|x\|\|x'\|}$. $J_n(\theta) = (-1)^n \sin^n (\theta) + 1 \left(\frac{n}{\pi x\theta}\right)^n$.

where $V = (v_1(\cdot), \ldots, v_k(\cdot))$ is the top $k$ eigenfunctions of $A$, and $\Sigma_k$ is a diagonal matrix with the corresponding eigenvalues, $V_{\perp}$ is the collection of the rest of the eigenfunctions, and $\Sigma_{\perp}$ is a diagonal matrix with the rest of the eigenvalues.

In the finite data case, the empirical covariance operator is $A = \frac{1}{n} \sum_x k(x, \cdot)k(x, \cdot)^\top$ or denoted as $\frac{1}{n} \sum_i k(x_i, \cdot) \odot k(x_i, \cdot)$. According to the representer theorem, the solutions of the top $k$ eigenfunctions of $A$ can be expressed as linear combinations of the training points with the set of coefficients $\{\alpha_i\}_{i=1}^k \in \mathbb{R}^n$, $v_i = \sum_{j=1}^n \alpha_j^i k(x_j, \cdot)$

Using $A v(\cdot) = \lambda v(\cdot)$ and the kernel trick, we have

$$K \alpha_i = \lambda_i \alpha_i,$$

where $K$ is the $n \times n$ Gram matrix.

The infinite dimensional problem is thus reduced to a finite dimensional eigenvalue problem. However, this dual approach is clearly impractical on large scale datasets due quadratic memory and computational costs.

### 3.3 Random feature approximation

The usage of random features to approximate a kernel function is motivated by the following theorem.

**Theorem 1** (Bochner). A continuous, real-valued, symmetric and shift-invariant function $k(x - x')$ on $\mathbb{R}^d$ is a PD kernel if and only if there is a finite non-negative measure $\mathbb{P}(\omega)$ on $\mathbb{R}^d$, such that $k(x - x') = \int_{\mathbb{R}^d} e^{i\omega^\top (x-x')} d\mathbb{P}(\omega) = \int_{\mathbb{R}^d} [0, 2\pi e] \phi_\omega(x) \phi_\omega(y) d(\mathbb{P}(\omega) \times \mathbb{P}(b))$, where $\mathbb{P}(b)$ is a uniform distribution on $[0, 2\pi]$, and $\phi_\omega(x) = \sqrt{2} \cos(\omega^\top x + b)$.

The theorem says that any shift-invariant kernel function $k(x, y) = k(x - y)$, e.g., Gaussian RBF kernel, can be considered as an expectation of two feature functions $\phi_\omega(x)$ and $\phi_\omega(y)$, where the expectation is taken over a distribution on the random frequency $\omega$ and phase $b$.

We can therefore approximate the kernel function as an empirical average of samples from the distribution. In other words,

$$k(x, y) \approx \frac{1}{B} \sum_i \phi_\omega(x) \phi_\omega(y),$$
where \( \{(\omega_i, b_i)\}_{i=1}^{B} \) are i.i.d. samples drawn from \( \mathbb{P}(\omega) \) and \( \mathbb{P}(b) \), respectively.

The specific random feature functions and distributions have been worked out for many popular kernels. For Gaussian RBF kernel, \( k(x, x') = \exp(-\|x - x'\|^2/2\sigma^2) \), this yields a Gaussian distribution \( \mathbb{P}(\omega) \) with density proportional to \( \exp(-\sigma^2\|\omega\|^2/2) \); for the Laplace kernel, this yields a Cauchy distribution; and for the Martern kernel, this yields the convolutions of the unit ball [27]. Similar representation where the explicit form of \( \phi(\omega) \) and \( \mathbb{P}(\omega) \) are known can also be derived for rotation invariant kernel, \( k(x, x') = k(\langle x, x' \rangle) \), using Fourier transformation on sphere [27]. For polynomial kernels, \( k(x, x') = (\langle x, x' \rangle + c)^p \), a random tensor sketching approach can also be used [22]. See Table 1 for explicit representations of different kernels.

4 Algorithm

In this section, we will design efficient algorithm based on the “doubly stochastic gradients” to scale up kernel PCA. The kernel PCA problem is essentially the eigenvalue problem in a functional space. This can be formulated as the following non-convex optimization problem

\[
\begin{align*}
\max_{G} & \quad \text{tr} (G^T AG) \\
\text{s.t.} & \quad G^T G = I
\end{align*}
\]

where \( G := (g^1, \ldots, g^k) \) and \( g^i \) is the \( i \)-th function.

The Lagrangian that incorporates the constraint is

\[
L(G, \Lambda) = \text{tr} (G^T AG) + \text{tr} ((G^T G - I) \Lambda)
\]

where \( \Lambda \) is the Lagrangian multiplier. The gradient of the Lagrangian w.r.t \( G \)

\[
\nabla_G L = 2AG + G (\Lambda + \Lambda^T) .
\]

Furthermore, from the optimality conditions

\[
2AG + G (\Lambda + \Lambda^T) = 0,
\]

\[
G^T G - I = 0,
\]

we can find \( \Lambda + \Lambda^T = -2G^T AG \).

Plugging this into the gradient, it suggests the following update rule

\[
G_{t+1} = G_t + \eta_t (I - G_t G_t^T) AG_t .
\]

Since we do not have the expectation \( A \), we can use its empirical average over a mini-batch \( A_t \) in the update rule. Let \( \{x_1^t, x_2^t, \ldots, x_B^t\} \) be a mini-batch of \( B \) data points. Then the empirical covariance operator \( A_t : \mathcal{F} \mapsto \mathcal{F} \) is

\[
A_t f(\cdot) = \frac{1}{B} \sum_{i=1}^{B} f(x_i^t) k(x_i^t, \cdot), \quad \forall f \in \mathcal{F}
\]

and furthermore \( A = \mathbb{E}_x [A_t] \). For simplicity of notation, we assume only one data point \( x_t \) is used to approximate \( A \).

Denote the evaluation of \( G_t \) at the current data point as

\[
g_t = [g^1_t(x_t), \ldots, g^k_t(x_t)]^T \in \mathbb{R}^k .
\]

We have

\[
A_t G_t = k(x_t, \cdot) g_t^T
\]

\[
G_t^T A_t G_t = g_t g_t^T
\]
Algorithm 1: \( \{ \alpha_i \}^t_1 = \text{DSGD-KPCA}(P(x), k) \)

Require: \( P(\omega), \phi_\omega(x) \).

1: for \( i = 1, \ldots, t \) do
2:  Sample \( x_i \sim P(x) \).
3:  Sample \( \omega_i \sim P(\omega) \) with seed \( i \).
4:  \( h_i = \text{Evaluate} \left( x_i, \{ \alpha_j \}^i_1 \right) \in \mathbb{R}^k \).
5:  \( \alpha_i = \eta_i \phi_\omega(x_i) h_i \).
6:  \( \alpha_j = \alpha_j - \eta_i \alpha_j^\top h_i h_i \), for \( j = 1, \ldots, i - 1 \).
7: end for

Therefore, the update rule can be re-written as

\[
G_{t+1} = G_t \left( I - \eta_t g_t g_t^\top \right) + \eta_t k(x_t, \cdot) g_t^\top.
\]

This rule can also be derived by using stochastic gradient and Oja’s rule without orthogonalization \cite{20, 21}.

Though a classic and popular tool, this update rule has a fundamental computational drawback. At each time step \( t \), a new basis \( k(x_t, \cdot) \) is added to \( G_t \), and it is therefore a linear combination of the feature mappings of all the data points up to \( t \). This requires the algorithm to store all the data points it has seen so far, which is impractical for large scale datasets.

To tackle this issue, we use the random feature approximation

\[
k(x, \cdot) = \mathbb{E} \left[ \phi_\omega(x) \phi_\omega(\cdot) \right] \approx \frac{1}{B} \sum_i \phi_\omega_i(x) \phi_\omega_i(\cdot),
\]

where \( \omega_i \) are sampled from the distribution \( p(\omega) \) associated with the kernel function.

Again, for simplicity of notation, we assume at each time, we only use one random feature to approximate the kernel function.

\[
H_{t+1} = H_t \left( I - \eta_t h_t h_t^\top \right) + \eta_t \phi_\omega(x_t) \phi_\omega(\cdot) h_t^\top,
\]

where \( h_t \) is the evaluation of \( H_t \) at the current data point:

\[
h_t = [h_t^1(x_t), \ldots, h_t^k(x_t)]^\top \in \mathbb{R}^k.
\]

Given \( H_0 = V_0 \), we can explicitly represent \( H_t \) as a linear combination of all the random feature functions \( \phi_\omega(\cdot) \):

\[
H_t = \sum_i \phi_\omega_i(\cdot) \alpha_i^\top + V_0 \beta,
\]

where \( \alpha_i \in \mathbb{R}^k \) are the coefficients, and \( \beta = \prod_{i \leq t} \left( I - \eta_i h_i h_i^\top \right) \).

The update rule on the functions corresponds to the following update for the coefficients

\[
\alpha_{t+1} = \eta_t \phi_\omega(x_t) h_t \quad \quad \alpha_i = \alpha_i - \eta_i \alpha_i^\top h_i h_i, \quad \forall i \leq t.
\]

The specific updates are also summarized in Algorithms 1 and 2.

5 Analysis

In order to analyze the convergence of our doubly stochastic kernel PCA algorithm, we will need to define a few intermediate subspaces. For simplicity of notation, we will assume the mini-batch size for the data points is one.
Algorithm 2: $h = \text{Evaluate}(x, \{\alpha_i\}_{i=1}^{t})$

Require: $P(\omega), \phi_\omega(x)$.

1. Set $h = 0 \in R^k$.

2. for $i = 1, \ldots, t$ do

3. Sample $\omega_i \sim P(\omega)$ with seed $i$.

4. $h = h + \phi_{\omega_i}(x)\alpha_i$.

5. end for

1. Let $F_t := \{f_1^t, \ldots, f_k^t\}$ be the subspace estimated using stochastic gradient and explicit orthogonalization:

\[
\hat{F}_{t+1} \leftarrow F_t + \eta_t A_t F_t
\]

\[
F_{t+1} \leftarrow \hat{F}_{t+1} \left(\hat{F}_{t+1}^\top \hat{F}_{t+1}\right)^{-1/2}
\]

2. Let $G_t := \{g_1^t, \ldots, g_k^t\}$ be the subspace estimated using stochastic update rule without orthogonalization:

\[
G_{t+1} \leftarrow G_t + \eta_t \left(I - G_t G_t^\top\right) A_t G_t.
\]

where $A_t G_t$ and $G_t G_t^\top A_t G_t$ can be equivalently written using the evaluation of the function $\{g_i^t\}$ on the current data point, leading to the equivalent rule:

\[
G_{t+1} \leftarrow G_t \left(I - \eta_t g_t g_t^\top\right) + \eta_t k(x_t, \cdot) g_t^\top.
\]  \hfill (15)

3. Let $\tilde{G}_t := \{\tilde{g}_1^t, \ldots, \tilde{g}_k^t\}$ be the subspace estimated using stochastic update rule without orthogonalization, but the evaluation of the function $\{\tilde{g}_i^t\}$ on the current data point is replaced by the evaluation $h_t = [h_i^t(x_t)]^\top$:

\[
\tilde{G}_{t+1} \leftarrow \tilde{G}_t + \eta_t k(x_t, \cdot) h_t^\top - \eta_t \tilde{G}_t h_t h_t^\top.
\]

4. Let $H_t := \{h_1^t, \ldots, h_k^t\}$ be the subspace estimated using doubly stochastic update rule without orthogonalization, i.e., the update rule:

\[
H_{t+1} \leftarrow H_t + \eta_t \omega_i(x_t)\phi_\omega(\cdot) h_t^\top - \eta_t H_t h_t h_t^\top.
\]  \hfill (16)

The relation of these subspaces are summarized in Table 2. Using these notations, we describe a sketch of our analysis in the rest of the section, while the complete proofs are provided in the appendix.

We first consider the subspace $G_t$ estimated using the stochastic update rule, since it is simpler and its proof can provide the bases for analyzing the subspace $H_t$ estimated by the doubly stochastic update rule.

| Subspace | Evaluation | Orth. | Data Mini-batch | RF Mini-batch |
|----------|------------|-------|-----------------|---------------|
| $V$      | -          | -     | -               | -             |
| $F_t$    | $f_t(x)$   | ✓     | ✓               | x             |
| $G_t$    | $g_t(x)$   | x     | ✓               | x             |
| $\tilde{G}_t$ | $h_t(x)$ | x     | ✓               | x             |
| $H_t$    | $h_t(x)$   | x     | ✓               | ✓             |
5.1 Stochastic update

Our guarantee is on the cosine of the principal angle between the computed subspace and the ground truth eigen subspace $V$ (also called the potential function), which is a standard criterion for measuring the quality of the subspace:

$$\cos^2 \theta(V, G_t) = \min_w \frac{\|V^T G_t w\|^2}{\|G_t w\|^2}.$$ 

We will focus on the case when a good initialization $V_0$ is given:

$$V_0^T V_0 = I, \quad \cos^2 \theta(V, V_0) \geq 1/2.$$ (17)

In other words, we analyze the later stage of the convergence, which is typical in the literature (e.g., [32]). The early stage can be analyzed using established techniques (e.g., [6]).

We will also focus on the dependence of the potential function on the step $t$. For this reason, throughout the paper we suppose $|k(x, x')| \leq \kappa, |\phi_0(x)| \leq \phi$ and regard $\kappa$ and $\phi$ as constants. Note that this is true for all the kernels and corresponding random features considered. We further regard the eigengap $\lambda_k - \lambda_{k+1}$ as a constant, which is also true for typical applications and datasets. Details can be found in the appendix.

Our final guarantee for $G_t$ is stated in the following.

**Theorem 2.** Assume [17] and suppose the mini-batch sizes satisfy that for any $1 \leq i \leq t$, $\|A - A_i\| < (\lambda_k - \lambda_{k+1})/8$. There exist step sizes $\eta_i = O(1/i)$ such that

$$1 - \cos^2 \theta(V, G_t) = O(1/t).$$

The convergence rate $O(1/t)$ is in the same order as that when computing only the top eigenvector in linear PCA [6], though we are not aware of any other convergence rate for computing the top $k$ eigenfunctions in Kernel PCA. The bound requires the mini-batch sizes are large enough so that the spectral norm of $A$ is approximated up to the order of the eigengap. This is due to the fact that approximating $A$ with $A_t$ will result in an error term in the order of $\|A - A_t\|$, while the increase of the potential is in the order of the eigengap. Similar terms appear in the analysis of the noisy power method [14], which, however, requires normalization and is not suitable for the kernel case. We do not specify the mini-batch sizes, but by assuming suitable data distributions, it is possible to obtain explicit bounds; see for example [34, 7].

**Proof sketch** We first prove the guarantee for the normalized subspace $F_t$ which is more convenient to analyze, and then show that the updates for $F_t$ and $G_t$ are first order equivalent so $G_t$ enjoys the same guarantee.

**Lemma 3.** $1 - \cos^2 \theta(V, F_t) = O(1/t)$.

Let $c_i^2$ denote $\cos^2 \theta(V, F_i)$, then a key step in proving the lemma is to show the following recurrence

$$c_{t+1}^2 \geq c_t^2(1 + 2\eta_t(\lambda_k - \lambda_{k+1} - 2\|A - A_t\|)(1 - c_t^2)) - O(\eta_t^2).$$ (18)

Therefore, we will need the mini-batch sizes large enough so that $2\|A - A_t\|$ is smaller than the eigen-gap.

Another key element in the proof of the theorem is the first order equivalence of the two update rules. To show this, we need to compare the subspaces obtained by applying the them on the same subspace $G_t$. So we introduce $F(G_t)$ to denote the subspace by applying the update rule of $F_t$ on $G_t$:

$$\tilde{F}(G_t) \leftarrow G_t + \eta_t A_t G_t$$

$$F(G_t) \leftarrow \tilde{F}(G_t) \left[\tilde{F}(G_t)^\top \tilde{F}(G_t)\right]^{-1/2}$$

We show that the potentials of $G_{t+1}$ and $F(G_t)$ are close.

**Lemma 4.** $\cos^2 \theta(V, G_{t+1}) = \cos^2 \theta(V, F(G_t)) \pm O(\eta_t^2)$. 

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The lemma means that applying the two update rules to the same input will result in two subspaces with similar potentials. Since \( \cos^2 \theta(V, F(G_i)) \) enjoys the recurrence in (18), we know that \( \cos^2 \theta(V, G_{t+1}) \) also enjoys such a recurrence, which then results in \( 1 - \cos^2 \theta(V, G_i) = O(1/t) \).

The proof of the lemma is based on the observation that

\[
\cos^2 \theta(V, X) = \lambda_{\min}(V^T X (X^T X)^{-1} X^T V).
\]

The lemma follows by plugging in \( X = G_{t+1} \) or \( X = F(G_t) \) and comparing their Taylor expansions w.r.t. \( \eta_t \).

### 5.2 Doubly stochastic update

For doubly stochastic update rule, the computed \( H_t \) is no longer in the RKHS so the principal angle is not well defined. Since the eigenfunction \( v \) is usually used for evaluating on points \( x \), we will use the following point-wise convergence in our analysis. For any function \( v \) in the subspace of \( V \) with unit norm \( ||v||_F = 1 \), we will find a specially chosen function \( h \) in the subspace of \( H_t \) such that for any \( x \),

\[
\text{err} := |v(x) - h(x)|^2
\]

is small with high probability. More specifically, the \( w \) is chosen to be \( \tilde{G}_t^\top v \), and let \( \tilde{g} = \tilde{G}_t w \) and \( h = H_t w \). Then the error measure can be decomposed as

\[
|v(x) - h(x)|^2 = |v(x) - \tilde{g}(x) + \tilde{g}(x) - h(x)|^2 \\
\leq 2|v(x) - \tilde{g}(x)|^2 + 2|\tilde{g}(x) - h(x)|^2 \\
\leq 2\kappa^2 \|v - \tilde{g}\|_F^2 + 2\|\tilde{g}(x) - h(x)\|^2. \tag{19}
\]

The distance \( \|v - \tilde{g}\|_F \) is closely related to the squared sine of the subspace angle between \( V \) and \( \tilde{G}_t \). In fact, by definition, \( \|v - \tilde{g}\|_F^2 = \|v\|_F^2 - \|\tilde{g}\|_F^2 \leq 1 - \cos^2 \theta(V, \tilde{G}_t) \). Therefore, the first error term can be bounded by the guarantee on \( \tilde{G}_t \), which can be obtained by similar arguments as for the stochastic update case. For the second term, note that \( \tilde{G}_t \) is defined in such a way that the difference between \( \tilde{g}(x) = \tilde{G}_t(x)w \) and \( h(x) = H_t(x)w \) is a martingale, which can be bounded by careful analysis.

Overall, we have the following results. Suppose we use random Fourier features; see [23]. Similar bounds hold for other random features, where the batch sizes will depend on the concentration bound of the random features used.

**Theorem 5.** Assume (17) and suppose the mini-batch sizes satisfy that for any \( 1 \leq i \leq t \), \( \|A - A_i\| < (\lambda_k - \lambda_{k+1})/8 \) and are of order \( \Omega(\ln \frac{1}{\delta}) \). There exist step sizes \( \eta_i = O(1/i) \), such that the following holds. If \( \Omega(1) = \lambda_k(\tilde{G}_t^\top \tilde{G}_i) \leq \lambda_1(\tilde{G}_t^\top \tilde{G}_i) = O(1) \) for all \( 1 \leq i \leq t \), then for any \( x \) and any function \( v \) in the span of \( V \) with unit norm \( ||v||_F = 1 \), we have that with probability \( \geq 1 - \delta \), there exists \( h \) in the span of \( H_t \) satisfying

\[
|v(x) - h(x)|^2 = O \left( \frac{1}{t} \ln \frac{t}{\delta} \right).
\]

The point-wise error scales as \( \tilde{O}(1/t) \) with the step \( t \), which is in similar order as that for the stochastic update rule. Again, we require the spectral norm of \( A \) to be estimated up to the order of the eigengap, for the same reason as before. We additionally need that the random features approximate the kernel function up to constant accuracy on all the data points up to time \( t \), since the evaluation of the kernel function on these points are used in the update. This eventually leads to \( \Omega(\ln \frac{1}{\delta}) \) mini-batch sizes. Finally, we need \( \tilde{G}_t^\top \tilde{G}_i \) to be roughly isotropic, i.e., \( \tilde{G}_i \) is roughly orthonormal. Intuitively, this should be true for the following
reasons: \( \tilde{G}_0 \) is orthonormal; the update for \( \tilde{G}_t \) is close to that for \( G_t \), which in turn is close to \( F_t \) that are orthonormal.

**Proof sketch** The analysis is carried out by bounding each term in (19) separately. As discussed above, in order to bound term I, we need a bound on the squared cosine of the subspace angle between \( V \) and \( \tilde{G}_t \).

**Lemma 6.** \( 1 - \cos^2 \theta(V, \tilde{G}_t) = O \left( \frac{1}{t} \ln \frac{1}{\delta} \right) \).

To prove this lemma, we follow the argument for Theorem 2 and get the recurrence as shown in (18), except with an additional error term, which is caused by the fact that the update rule for \( \tilde{G}_{t+1} \) is using the evaluation \( h_t(x_t) \) rather than \( \tilde{g}_t(x_t) \). Bounding this additional term thus relies on bounding the difference between \( h_t(x) - \tilde{g}_t(x) \), which is also what we need for bounding term II in (19). For this purpose, we show the following bound:

**Lemma 7.** For any \( x \) and unit vector \( w \), with probability \( \geq 1 - \delta \) over \((D^t, \omega^t)\), \( |\tilde{g}_t(x) w - h_t(x) w|^2 = O \left( \frac{1}{t} \ln \left( \frac{1}{\delta} \right) \right) \).

The key to prove this lemma is that our construction of \( \tilde{G}_t \) makes sure that the difference between \( \tilde{g}_t(x) w \) and \( h_t(x) w \) consists of their difference in each time step. Furthermore, the difference in each time step conditioned on previous history has mean 0. In other words, the difference forms a martingale and thus can be bounded by Azuma’s inequality. The resulting bound depends on the mini-batch sizes, the step sizes \( \eta_t \), and the evaluations \( h_t(x_t) \) used in the update rules. We then judiciously choose the parameters and simplify it to the bound in the lemma. The complication of the proof is mostly due to the interweaving of the parameter values; see the appendix for the details.

### 6 Extensions

The proposed algorithm is a general technique for solving eigenvalue problems in the functional space. Numerous machine learning algorithms boil down to this fundamental operation. Therefore, our method can be easily extended to solve many related tasks, including latent variable estimation, kernel CCA, spectral clustering, etc.

We briefly illustrate how to extend to different machine learning algorithms in the following subsections.

#### 6.1 Locating individual eigenfunctions

The proposed algorithm finds the subspace spanned by the top \( k \) eigenfunctions, but it does not isolate the individual eigenfunctions. When we need to locate these individual eigenfunctions, we can use a modified version, called Generalized Hebbian Algorithm (GHA) [26]. Its update rule is

\[
G_{t+1} = G_t + \eta_t A_t G_t - \eta_t G_t U^T [G^T_t A_t G_t],
\]

where \( U^T \cdot \) is an operator that sets the lower triangular parts to zero.

To understand the effect of the upper triangular operator, we can see that \( U^T \cdot \) forces the update rule for the first function of \( G_t \) to be exactly the same as that of one-dimensional subspace; all the contributions from the other functions are zeroed out.

\[
g_{1,t+1} = g_{1,t} + \eta_t A_t g_{1,t} - \eta_t g_{1,t} g_{1,t}^T A_t g_{1,t},
\]

Therefore, the first function will converge to the eigenfunction corresponding to the top eigenvalue.

For all the other functions, \( U^T \cdot \) implements a Gram-Schmidt-like orthogonalization that subtracts the contributions from other eigenfunctions.
Algorithm 3: \( \{\alpha_i, \beta_i\}_i^T = \text{DSGD-KSVD}(\mathbb{P}(x), \mathbb{P}(y), k) \)

Require: \( \mathbb{P}(\omega), \phi_\omega(x) \).

1: for \( i = 1, \ldots, t \) do
2: Sample \( x_i \sim \mathbb{P}(x) \). Sample \( y_i \sim \mathbb{P}(y) \).
3: Sample \( \omega_i \sim \mathbb{P}(\omega) \) with seed \( i \).
4: \( u_i = \text{Evaluate}(x_i, \{\alpha_j\}_{j=1}^{i-1}) \in \mathbb{R}^k \).
5: \( v_i = \text{Evaluate}(y_i, \{\beta_j\}_{j=1}^{i-1}) \in \mathbb{R}^k \).
6: \( W = u_i v_i^T + v_i u_i^T \).
7: \( \alpha_i = \eta_i \phi_\omega(x_i) v_i \).
8: \( \beta_i = \eta_i \phi_\omega(y_i) u_i \).
9: \( \alpha_j = \alpha_j - \eta_i W \alpha_j \), for \( j = 1, \ldots, i - 1 \).
10: \( \beta_j = \beta_j - \eta_i W \beta_j \), for \( j = 1, \ldots, i - 1 \).
11: end for

6.2 Latent variable models and kernel SVD

Latent variable models are probabilistic models that assume unobserved or latent structures in the data. It appears in specific forms such as Gaussian Mixture Models (GMM), Hidden Markov Models (HMM) and Latent Dirichlet Allocations (LDA), etc.

The EM algorithm \cite{12} is considered the standard approach to solve such models. Recently, spectral methods have been proposed to estimate latent variable models with provable guarantees \cite{2, 33}. Compared with the EM algorithm, spectral methods are faster to compute and do not suffer from local optima.

The key algorithm behind spectral methods is the SVD. However, kernel SVD scales quadratically with the number of data points. Our algorithm can be straightforwardly extended to solve kernel SVD. The extension hinges on the following relation

\[
\begin{bmatrix}
0 & A^T \\
A & 0
\end{bmatrix}
\begin{bmatrix}
V \\
U
\end{bmatrix}
= 
\begin{bmatrix}
A^T U \\
V
\end{bmatrix}
\Sigma,
\]

where \( U \Sigma V^T \) is the SVD of \( A \).

It is therefore reduced to the eigenvalue problem. Plugging it into the update rule and treating the two blocks separately, we thus get two simultaneous update rules

\[
W_t = U_t^T AV_t + V_t^T A^T U_t,
\]

\[
U_{t+1} = U_t + \eta_t (AV_t - U_t W_t),
\]

\[
V_{t+1} = V_t + \eta_t (A^T U_t - V_t W_t).
\]

The algorithm for updating the coefficients is summarized in Algorithm 3.

6.3 Kernel CCA and generalized eigenvalue problem

Kernel CCA and ICA \cite{4} can also be solved under the proposed framework because they can be viewed as generalized eigenvalue problem.

Given two variables \( X \) and \( Y \), CCA finds two projections such that the correlations between the two projected variables are maximized. Given the covariance matrices \( C_{XX}, C_{YY}, \) and \( C_{XY} \), CCA is equivalent to the following problem

\[
\begin{bmatrix}
C_{XX} & C_{XY} \\
C_{YX} & C_{YY}
\end{bmatrix}
\begin{bmatrix}
g_X \\
g_Y
\end{bmatrix}
= (1 + \sigma^2)
\begin{bmatrix}
C_{XX} & C_{XY} \\
C_{YX} & C_{YY}
\end{bmatrix}
\begin{bmatrix}
g_X \\
g_Y
\end{bmatrix},
\]

where \( g_X \) and \( g_Y \) are the top canonical correlation functions for variables \( X \) and \( Y \), respectively, and \( \sigma \) is the corresponding canonical correlation.
Algorithm 4: $\{\alpha_i, \beta_i\}_{i=1}^t = \text{DSGD-KCCA}(\mathbb{P}(x), \mathbb{P}(y), k)$

Require: $\mathbb{P}(\omega), \phi_\omega(x)$.

1: for $i = 1, \ldots, t$ do
2: Sample $x_i \sim \mathbb{P}(x)$. Sample $y_i \sim \mathbb{P}(y)$.
3: Sample $\omega_i \sim \mathbb{P}(\omega)$ with seed $i$.
4: $u_i = \text{Evaluate}(x_i, \{\alpha_j\}_{j=1}^{i-1}) \in \mathbb{R}^k$.
5: $v_i = \text{Evaluate}(y_i, \{\beta_j\}_{j=1}^{i-1}) \in \mathbb{R}^k$.
6: $W = u_i v_i^\top + v_i u_i^\top$.
7: $\alpha_i = \eta_i \phi_\omega(x_i) [v_i - W u_i]$.
8: $\beta_i = \eta_i \phi_\omega(y_i) [u_i - W v_i]$.
9: end for

This is a generalized eigenvalue problem. It can reformulated as the following non-convex optimization problem

$$\max_G \text{tr} \left( G^\top A G \right),$$

s.t. $G^\top B G = I$. (25)

Following the derivation for the standard eigenvalue problem, we get the following update rules

$$G_{t+1} = G_t + \eta_t \left( I - B G_t G_t^\top \right) A G_t.$$ (27)

Denote $G^X_t$ and $G^Y_t$ the canonical correlation functions for $X$ and $Y$, respectively. We can rewrite the above update rule as two simultaneous rules

$$W_t = G_t^Y C_{YX} G_t^X + G_t^X C_{XY} G_t^Y,$$ (28)

$$G_{t+1}^X = G_t^X + \eta_t \left[ C_{XY} G_t^Y - C_{XX} G_t^X W \right]$$ (29)

$$G_{t+1}^Y = G_t^Y + \eta_t \left[ C_{YX} G_t^X - C_{YY} G_t^Y W \right].$$ (30)

We present the detailed updates for coefficients in Algorithm 4.

6.4 Other extensions

Spectral clustering has been shown to be equivalent to first doing KPCA and then perform $k$-means algorithms on the embedding (e.g., [13]).

7 Experiments

We demonstrate the effectiveness and scalability of our algorithm on both synthetic and real world datasets.

7.1 Synthetic dataset with analytical solution

We first verify the convergence rate of DSGD-KPCA on a synthetic dataset with analytical solution of eigenfunctions [35]. If the data follow a Gaussian distribution, and we use a Gaussian kernel, then the eigenfunctions are given by the Hermite polynomials.

We generated 1 million data points, and ran DSGD-KPCA with a total of 262,144 random features. In each iteration, we use a data mini-batch of size 512, and a random feature mini-batch of size 128. After all random features are generated, we revisit and adjust the coefficients of existing random features. The kernel bandwidth is set as the true bandwidth of the data.
The step size is scheduled as

\[ \eta_t = \frac{\theta_0}{1 + \theta_1 t}, \]  \hspace{1cm} (31)

where \( \theta_0 \) and \( \theta_1 \) are two parameters. We use a small \( \theta_1 \approx 0.01 \) such that in early stages the step size is large enough to arrive at a good initial solution.

**Convergence** Figure 1 shows the convergence rate of the proposed algorithm seeking top \( k = 3 \) subspace. The potential function is calculated as the squared sine function of the subspace angle between the current solution and the ground-truth. We can see the algorithm indeed converges at the rate \( O(1/t) \).

**Eigenfunction Recovery** Figure 2 demonstrate the recovered top \( k = 3 \) eigenfunctions compared with the ground-truth. We can see the found solution coincides with one eigenfunction, and only disagree slightly on two others.

### 7.2 Nonparametric Latent Variable Model

In [33], the authors proposed a multiview nonparametric latent variable model that is solved by kernel SVD followed by tensor power iterations. The algorithm can separate latent variables without imposing specific parametric assumptions of the conditional probabilities. However, the scalability of the algorithm was limited by kernel SVD.
Table 3: KCCA results on MNIST 8M (top 50 largest correlations)

| # of feat | Random features | Nystrom features |
|-----------|-----------------|------------------|
|           | corrs. | minutes | corrs. | minutes |
| 256       | 25.2   | 3.2     | 30.4   | 3.0     |
| 512       | 30.7   | 7.0     | 35.3   | 5.1     |
| 1024      | 35.3   | 13.9    | 38.0   | 10.1    |
| 2048      | 38.8   | 54.3    | 41.1   | 27.0    |
| 4096      | 41.5   | 186.7   | 42.7   | 71.0    |

Here, we demonstrate that with DSGD-KSVD, we can learn latent variable models with one million data, achieving higher quality of learned components compared with two other approaches.

DSGD-KSVD uses a total of 8192 random features, and in each iteration, it uses a feature mini-batch of size 256 and a data mini-batch of size 512.

We compare with 1) random Fourier features with fixed 2048 functions, and 2) random Nystrom features with fixed 2048 functions. The Nystrom features are calculated by first uniformly sampling 2048 data points, and then evaluate kernel function values on these data points [19].

The dataset consists of two latent components, one is a Gaussian distribution and the other follows a Gamma distribution with shape parameter $\alpha = 1.2$. One million data point are generated from this mixture distribution.

Figures 3 shows the learned conditional distributions for each component. We can see DSGD-KSVD achieves almost perfect recovery, while Fourier and Nystrom random feature methods either confuse high density areas or incorrectly estimate the spread of conditional distributions.

### 7.3 KCCA MNIST8M

We then demonstrate the scalability and effectiveness of our algorithm on a large-scale real world dataset. MNIST8M consists of 8.1 million hand-written digits and their transformations. Each digit is of size $28 \times 28$.

We divide each image into the left and right parts, and learn their correlations using KCCA. Thus the input feature dimension is 392.

The evaluation criteria is the total correlations on the top $k = 50$ canonical correlation directions calculated on a separate test set of size 10000. Out of the 8.1 million training data, we randomly choose 10000 as an evaluation set.

We compare with 1) random Fourier and 2) random Nystrom features on both total correlation and running time. We vary the number of random features used for both methods. Our algorithm uses a total of 20480 features. In each iteration, we use feature mini-batches of size 2048 and data mini-batches of size 1024, and we run 3000 iterations. The kernel bandwidth is set using the “median” trick and is the same for all methods. Due to randomness, all algorithms are run 5 times, and the mean is reported.

The results are presented in Table 3. We can see Nystrom features generally achieve better results than Fourier features. Note that for Fourier features, we are using the version with sin and cos pairs, so the real number of parameters is twice the number in the table, as a result the computational time is almost twice of that for Nystrom features.

Our algorithm achieves the best test-set correlations in comparable run time with random Fourier features. This is especially significant for random Fourier features, since the run time would increase by almost four times if double the number of features were used. We can also see that for large datasets, it is important to use more random features for better performance. Actually, the number of random features required should grow linearly with the number of data points. Therefore, our algorithm provides a good balance between...
Figure 3: Recovered latent components (a) DSGD-KSVD, (b) 2048 random features, (c) 2048 Nystrom features.
the number of random features used and the number of data points processed.

8 Conclusions

We have proposed a general and scalable approach to solve nonlinear component analysis based on doubly stochastic gradients. It is simple, efficient and scalable. In addition, we have theoretical guarantees that the whole subspace converges at the rate $\tilde{O}(1/t)$ to the true subspace. Moreover, since its core is an algorithm for eigenvalue problems in the functional space, it can be applied to various other tasks and models. Finally, we demonstrate the scalability and effectiveness of our algorithm on both synthetic and real world datasets.

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Appendix

The appendix is organized as follows. Section A reviews notations, the definition of Kernel PCA and the update rules considered. Section B provides the sketch of the proof as in the paper. Section C provides the proof for the stochastic update rule, and Section D provides the proof for the doubly stochastic update rule.

A Setting

Notations Given a distribution \( P(x) \), a kernel function \( k(x, x') \) with RKHS \( \mathcal{F} \), the covariance operator \( A : \mathcal{F} \mapsto \mathcal{F} \) is a linear self-adjoint operator defined as

\[
Af(\cdot) := \mathbb{E}_x[f(x)k(x, \cdot)], \quad \forall f \in \mathcal{F},
\]

and furthermore

\[
\langle g, Af \rangle_{\mathcal{F}} = \mathbb{E}_x[f(x)g(x)], \quad \forall g \in \mathcal{F}.
\]

Let \( F = (f_1(\cdot), f_2(\cdot), \ldots, f_k(\cdot)) \) be a list of \( k \) functions in the RKHS, and we define matrix-like notation

\[
AF(\cdot) := (Af_1(\cdot), \ldots, Af_k(\cdot)),
\]

and \( F^\top AF \) is a \( k \times k \) matrix, whose \( (i, j) \)-th element is \( \langle f_i, Af_j \rangle_{\mathcal{F}} \). The outer-product of a function \( v \in \mathcal{F} \) defines a linear operator \( vv^\top : \mathcal{F} \mapsto \mathcal{F} \) such that

\[
(vv^\top)f(\cdot) := \langle v, f \rangle_{\mathcal{F}} v(\cdot), \quad \forall f \in \mathcal{F}
\]

Let \( V = (v_1(\cdot), \ldots, v_k(\cdot)) \) be a list of \( k \) functions, then the weighted sum of a set of linear operators, \( \{v_i v_i^\top \}_{i=1}^{k} \), can be denoted using matrix-like notation as

\[
V \Sigma_k V^\top := \sum_{i=1}^{k} \lambda_i v_i v_i^\top
\]

where \( \Sigma_k \) is a diagonal matrix with \( \lambda_i \) on the \( i \)-th entry of the diagonal.

Kernel PCA Kernel PCA aims to identify the top \( k \) eigenfunctions \( V = (v_1(\cdot), \ldots, v_k(\cdot)) \) for the covariance operator \( A \), where \( V \) is also called the top \( k \) subspace for \( A \).

A function \( v \) is an eigenfunction of covariance operator \( A \) with the corresponding eigenvalue \( \lambda \) if

\[
Av(\cdot) = \lambda v(\cdot).
\]

Given a set of eigenfunctions \( \{v_i\} \) and associated eigenvalues \( \{\lambda_i\} \), where \( \langle v_i, v_j \rangle_{\mathcal{F}} = \delta_{ij} \). We can denote the eigenvalue of \( A \) as

\[
A = V \Sigma_k V^\top + V_\perp \Sigma_\perp V_\perp^\top
\]

where \( V = (v_1(\cdot), \ldots, v_k(\cdot)) \) is the top \( k \) eigenfunctions of \( A \), and \( \Sigma_k \) is a diagonal matrix with the corresponding eigenvalues, \( V_\perp \) is the collection of the rest of the eigenfunctions, and \( \Sigma_\perp \) is a diagonal matrix with the rest of the eigenvalues.
### Update rules

The stochastic update rule is

$$ G_{t+1} = G_t + \eta_t \left( I - G_t G_t^\top \right) A_t G_t $$

where $G_t := (g^1_t, \ldots, g^k_t)$ and $g^i_t$ is the $i$-th function. Denote the evaluation of $G_t$ at the current data point as

$$ g_t = [g^1_t(x_t), \ldots, g^k_t(x_t)]^\top \in \mathbb{R}^k. $$

Then the update rule can be re-written as

$$ G_{t+1} = G_t \left( I - \eta_t g_t g_t^\top \right) + \eta_t k(x_t, \cdot) g_t^\top. $$

The doubly stochastic update rule is

$$ H_{t+1} = H_t \left( I - \eta_t h_t h_t^\top \right) + \eta_t \phi_{\omega_t}(x_t) \phi_{\omega_t}(\cdot) h_t^\top, $$

where $h_t$ is the evaluation of $H_t$ at the current data point:

$$ h_t = [h^1_t(x_t), \ldots, h^k_t(x_t)]^\top \in \mathbb{R}^k. $$

When larger mini-batch sizes are used, the update rule is adjusted accordingly. For example, when using $B_{x,t}$ points $\{x^b_t\}$ and $B_{\omega,t}$ features $\{\omega^b_t\}$, the update rule for $H_t$ is

$$ H_{t+1} \leftarrow H_t + \frac{\eta_t \sum_{b,b'} \phi_{\omega^b_t}(x^b_t) \phi_{\omega^{b'}_t}(\cdot) [h^1_t(x^b_t), \ldots, h^k_t(x^b_t)]}{B_{x,t} B_{\omega,t}} $$

$$ - \frac{\eta_t}{B_{x,t}} \sum_b \left[ h^1_t(x^b_t) h^b_t(x^b_t) \right]_{i,j=1}^k. $$

## B Analysis Roadmap

In order to analyze the convergence of our doubly stochastic kernel PCA algorithm, we will need to define a few intermediate subspaces. For simplicity of notation, we will assume the mini-batch size for the data points is one.

1. Let $F_t := (f^1_t, \ldots, f^k_t)$ be the subspace estimated using stochastic gradient and explicit orthogonalization:

   $$ \tilde{F}_{t+1} \leftarrow F_t + \eta_t A_t F_t $$

   $$ F_{t+1} \leftarrow \left( \tilde{F}_{t+1}^\top \tilde{F}_{t+1} \right)^{-1/2}. $$

2. Let $G_t := (g^1_t, \ldots, g^k_t)$ be the subspace estimated using stochastic update rule without orthogonalization:

   $$ G_{t+1} \leftarrow G_t + \eta_t \left( I - G_t G_t^\top \right) A_t G_t. $$

   where $A_t G_t$ and $G_t G_t^\top A_t G_t$ can be equivalently written using the evaluation of the function $\{g^i_t\}$ on the current data point, leading to the equivalent rule:

   $$ G_{t+1} \leftarrow G_t \left( I - \eta_t g_t g_t^\top \right) + \eta_t k(x_t, \cdot) g_t^\top. $$
3. Let $\tilde{G}_t := (\tilde{g}_1^t, \ldots, \tilde{g}_k^t)$ be the subspace estimated using stochastic update rule without orthogonalization, but the evaluation of the function $\{\tilde{g}_i\}$ on the current data point is replaced by the evaluation $h_t = [h_t^T(x_t)]^T$:

$$\tilde{G}_{t+1} \leftarrow \tilde{G}_t + \eta_t k(x_t, :)h_t^T - \eta_t \tilde{G}_t h_t h_t^T.$$ (46)

4. Let $H_t := (h_1^t, \ldots, h_k^t)$ be the subspace estimated using doubly stochastic update rule without orthogonalization, i.e., the update rule:

$$H_{t+1} \leftarrow H_t + \eta_t \phi_{w_t}(x_t)\phi_{w_t}(:)h_t^T - \eta_t H_t h_t h_t^T.$$ (47)

The relation of these subspaces are summarized in Table 4. Using these notations, we describe a sketch of our analysis in the rest of the section, while the complete proofs are provided in the following sections.

We first consider the subspace $G_t$ estimated using the stochastic update rule, since it is simpler and its proof can provide the bases for analyzing the subspace $H_t$ estimated by the doubly stochastic update rule.

Table 4: Relation between various subspaces.

| Subspace | Evaluation | Orth. | Data Mini-batch | RF Mini-batch |
|----------|------------|-------|-----------------|--------------|
| $V$      | –          | –     | –               | –            |
| $F_t$    | $f_t(x)$   | ✓     | ✓               | x            |
| $G_t$    | $g_t(x)$   | x     | ✓               | ✓            |
| $\tilde{G}_t$ | $h_t(x)$   | x     | ✓               | x            |
| $H_t$    | $h_t(x)$   | x     | ✓               | ✓            |

B.1 Stochastic update

Our guarantee is on the cosine of the principal angle between the computed subspace and the ground truth eigen subspace $V$ (also called the potential function), which is a standard criterion for measuring the quality of the subspace:

$$\cos^2 \theta(V, G_t) = \min_w \frac{\|V^T G_t w\|^2}{\|G_t w\|^2}.$$ (48)

We will focus on the case when a good initialization $V_0$ is given:

$$V_0^T V_0 = I, \quad \cos^2 \theta(V, V_0) \geq 1/2.$$ (49)

In other words, we analyze the later stage of the convergence, which is typical in the literature (e.g., [32]). The early stage can be analyzed using established techniques (e.g., [32]).

We will also focus on the dependence of the potential function on the step $t$. For this reason, throughout the paper we suppose $|k(x, x')| \leq \kappa, |\phi_{w_t}(x)| \leq \phi$ and regard $\kappa$ and $\phi$ as constants. Note that this is true for all the kernels and corresponding random features considered. We further regard the eigengap $\lambda_k - \lambda_{k+1}$ as a constant, which is also true for typical applications and datasets. Details can be found in the following sections.

Our final guarantee for $G_t$ is stated in the following.

**Theorem 2** Assume (48) and suppose the mini-batch sizes satisfy that for any $1 \leq i \leq t$, $\|A - A_i\| < (\lambda_k - \lambda_{k+1})/8$. There exist step sizes $\eta_i = O(1/i)$ such that

$$1 - \cos^2 \theta(V, G_t) = O(1/t).$$
The convergence rate $O(1/t)$ is in the same order as that when computing only the top eigenvector in linear PCA \cite{6}, though we are not aware of any other convergence rate for computing the top $k$ eigenfunctions in Kernel PCA. The bound requires the mini-batch sizes are large enough so that the spectral norm of $A$ is approximated up to the order of the eigengap. This is due to the fact that approximating $A$ with $A_t$ will result in an error term in the order of $\|A - A_t\|$, while the increase of the potential is in the order of the eigengap. Similar terms appear in the analysis of the noisy power method \cite{14} which, however, requires normalization and is not suitable for the kernel case. We do not specify the mini-batch sizes, but by assuming suitable data distributions, it is possible to obtain explicit bounds; see for example \cite{34,7}.

**Proof sketch** To prove the theorem, we first prove the guarantee for the normalized subspace $F_t$ which is more convenient to analyze, and then show that the update rules for $F_t$ and $G_t$ are first order equivalent so that $G_t$ enjoys the same guarantee.

**Lemma 3.** $1 - \cos^2 \theta(V, F_t) = O(1/t)$.

Let $c^2_t$ denote $\cos^2 \theta(V, F_t)$, then a key step in proving the lemma is to show that

$$c^2_{t+1} \geq c^2_t(1 + 2\eta_t(\lambda_k - \lambda_{k+1} - 2\|A - A_t\|(1 - c^2_t))) - O(\eta^2_t). \tag{49}$$

Therefore, we will need the mini-batch sizes large enough so that $2\|A - A_t\|$ is smaller than the eigen-gap.

Another key element in the proof of the theorem is the first order equivalence of the two update rules. To show this, we need to compare the subspaces obtained by applying the them on the same subspace $G_t$. So we introduce $F(G_t)$ to denote the subspace by applying the update rule of $F_t$ on $G_t$:

$$F(G_t) \leftarrow F(G_t) \leftarrow \tilde{F}(G_t) \leftarrow \tilde{F}(G_t) \leftarrow \left[\tilde{F}(G_t)^\top \tilde{F}(G_t)\right]^{-1/2}$$

We show that the potentials of $G_{t+1}$ and $F(G_t)$ are close:

**Lemma 4.** $\cos^2 \theta(V, G_{t+1}) = \cos^2 \theta(V, F(G_t)) \pm O(\eta^2_t)$.

The lemma follows by plugging in $X = G_{t+1}$ or $X = F(G_t)$ and comparing their Taylor expansions w.r.t. $\eta_t$.

**B.2 Doubly stochastic update**

For doubly stochastic update rule, the computed $H_t$ is no longer in the RKHS so the principal angle is not well defined. Since the eigenfunction $v$ is usually used for evaluating on points $x$, we will use the following point-wise convergence in our analysis. For any function $v$ in the subspace of $V$ with unit norm $\|v\|_V = 1$, we will find a specially chosen function $h$ in the subspace of $H_t$ such that for any $x$,

$$\text{err} := |v(x) - h(x)|^2$$
is small with high probability. More specifically, the $w$ is chosen to be $\hat{G}^\top v$, and let $\hat{g} = \hat{G}_t w$ and $h = H_t w$. Then the error measure can be decomposed as

\[
|v(x) - h(x)|^2 = |v(x) - \hat{g}(x) + \hat{g}(x) - h(x)|^2 \\
\leq 2|v(x) - \hat{g}(x)|^2 + 2|\hat{g}(x) - h(x)|^2 \\
\leq 2\kappa^2 \|v - \hat{g}\|^2_F + 2|\hat{g}(x) - h(x)|^2. \tag{50}
\]

The distance $\|v - \hat{g}\|^2_F$ is closely related to the squared sine of the subspace angle between $V$ and $\hat{G}_t$. In fact, by definition, $\|v - \hat{g}\|^2_F = \|v\|^2_F - \|\hat{g}\|^2_F \leq 1 - \cos^2 \theta(V, \hat{G}_t)$. Therefore, the first error term can be bounded by the guarantee on $\hat{G}_t$, which can be obtained by similar arguments as for the stochastic update case. For the second term, note that $\hat{G}_t$ is defined in such a way that the difference between $\hat{g}(x) = \hat{G}_t(x)w$ and $h(x) = H_t(x)w$ is a martingale, which can be bounded by careful analysis.

Overall, we have the following results. Suppose we use random Fourier features; see [23]. Similar bounds hold for other random features, where the batch sizes will depend on the concentration bound of the random features used.

**Theorem 5.** Assume [48] and suppose the mini-batch sizes satisfy that for any $1 \leq i \leq t$, $\|A - A_i\| < (\lambda_k - \lambda_{k+1})/8$ and are of order $\Omega(\ln t^2)$. There exist step sizes $\eta_i = O(1/i)$, such that the following holds. If $\Omega(1) = \lambda_k(\hat{G}_i^\top \hat{G}_i) \leq \lambda_1(\hat{G}_i^\top \hat{G}_i) = O(1)$ for all $1 \leq i \leq t$, then for any $x$ and any function $v$ in the span of $V$ with unit norm $\|v\|^2_F = 1$, we have that with probability $\geq 1 - \delta$, there exists $h$ in the span of $H_t$ satisfying

\[
|v(x) - h(x)|^2 = O \left( \frac{1}{t} \ln \frac{t}{\delta} \right).
\]

The point-wise error scales as $\tilde{O}(1/t)$ with the step $t$, which is in similar order as that for the stochastic update rule. Again, we require the spectral norm of $A$ to be estimated up to the order of the eigenfor, for the same reason as before. We additionally need that the random features approximate the kernel function up to constant accuracy on all the data points up to time $t$, since the evaluation of the kernel function on these points are used in the update. This eventually leads to $\Omega(\ln t^2)$ mini-batch sizes. Finally, we need $\hat{G}_t^\top \hat{G}_i$ to be roughly isotropic, i.e., $\hat{G}_i$ is roughly orthonormal. Intuitively, this should be true for the following reasons: $\hat{G}_0$ is orthonormal; the update for $\hat{G}_i$ is close to that for $\hat{G}_t$, which in turn is close to $F_i$ that are orthonormal.

**Proof sketch** The analysis is carried out by bounding each term in (50) separately. As discussed above, in order to bound term I, we need a bound on the squared cosine of the subspace angle between $V$ and $\hat{G}_t$.

**Lemma 6.** $1 - \cos^2 \theta(V, \hat{G}_t) = O \left( \frac{1}{t} \ln \frac{t}{\delta} \right)$.

To prove this lemma, we follow the argument for Theorem 2 and get the recurrence as shown in (49), except with an additional error term, which is caused by the fact that the update rule for $\hat{G}_{t+1}$ is using the evaluation $h_t(x_i)$ rather than $\hat{g}_t(x_i)$. Bounding this additional term thus relies on bounding the difference between $h_t(x) - \hat{g}_t(x)$, which is also what we need for bounding term II in (50). For this purpose, we show the following bound:

**Lemma 7.** For any $x$ and unit vector $w$, with probability $\geq 1 - \delta$ over $(D^t, \omega^t)$, $|\hat{g}_t(x)w - h_t(x)w|^2 = O \left( \frac{1}{t} \ln \frac{1}{\delta} \right)$.

The key to prove this lemma is that our construction of $\hat{G}_t$ makes sure that the difference between $\hat{g}_t(x)w$ and $h_t(x)w$ consists of their difference in each time step. Furthermore, the difference in each time step conditioned on previous history has mean 0. In other words, the difference forms a martingale and
thus can be bounded by Azuma’s inequality. The resulting bound depends on the mini-batch sizes, the step sizes $\eta_i$, and the evaluations $h_i(x_i)$ used in the update rules. We then judiciously choose the parameters and simplify it to the bound in the lemma. The complication of the proof is mostly due to the interweaving of the parameter values; see the following sections for the details.

C Stochastic Update

To prove the convergence of the stochastic update rule, we first prove the convergence of the normalized version $F_t$, and then we establish the first-order equivalence of the potential functions of the two update rules for $F_t$ and $G_t$. Since the final recurrence result does not depend on higher order terms, this first-order equivalence establishes the convergence of the stochastic update rule without normalization.

C.1 Stochastic update with normalization

We consider the potential function $1 - \cos^2 \theta (V,F_{t+1})$ and prove a recurrence for it. We first show this for the simpler case where at each step we use the expected operator $A$ in the update rule (Lemma 8), and then show this for the general case where $A_t$ can be different from $A$ (Lemma 9). Then the bound in Lemma 3 follows from solving the recurrence in Lemma 9.

C.1.1 Update rule with expected operator

The following lemma states the recurrence for the update rule which replace $A_t$ in the stochastic update rule with the expected operator $A = \mathbb{E}A_t$:

$$\tilde{F}_{t+1} \leftarrow F_t + \eta_t A F_t$$

$$F_{t+1} \leftarrow \tilde{F}_{t+1} \left( \tilde{F}_{t+1}^\top \tilde{F}_{t+1} \right)^{-1/2}$$

Lemma 8. Let the sequence $\{F_t\}_t$ be obtained from the update rule (51), then

$$1 - \cos^2 \theta (V,F_{t+1}) \leq \left[ 1 - \cos^2 \theta (V,F_t) \right] \left[ 1 - 2\eta_t (\lambda_k - \lambda_{k+1}) \cos^2 \theta (V,F_t) \right] + \beta_t,$$

where $\beta_t = 5\eta_t^2 B^2 + 3\eta_t^3 B^3$ and $\lambda_k$ and $\lambda_{k+1}$ are the top $k$ and $k+1$-th eigenvalues of $A$.

Proof. First note that the cosine of subspace angle does not change under linear combination of the basis

$$\cos^2 \theta (V,F_{t+1}) = \min_{w'} \frac{\| V^\top F_{t+1} w' \|^2}{\| F_{t+1} w' \|^2} = \min_{w'} \frac{\| V^\top \tilde{F}_{t+1} \left( \tilde{F}_{t+1}^\top \tilde{F}_{t+1} \right)^{-1/2} w' \|^2}{\| \tilde{F}_{t+1} \left( \tilde{F}_{t+1}^\top \tilde{F}_{t+1} \right)^{-1/2} w' \|^2} = \min_{w} \frac{\| V^\top \tilde{F}_{t+1} w \|^2}{\| \tilde{F}_{t+1} w \|^2}$$

The update rule gives us

$$\| V^\top \tilde{F}_{t+1} w \|^2 \geq \| V^\top F_t w \|^2 + 2\eta_t \langle V^\top F_t w, V^\top A F_t w \rangle$$

$$\| \tilde{F}_{t+1} w \|^2 \leq \| F_t w \|^2 + 2\eta_t \langle F_t w, A F_t w \rangle + B \| F_t w \|^2 \eta_t^2$$

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Let \( \dot{w} = w/\|F_tw\|, u = F_t\dot{w} \), so \( \|u\| = 1 \). Denote \( c = \|V^Tu\| \) and \( s = \|V^Tu_1\| \). According to the definition, we have \( c \geq \cos \theta_k (V, F_t) \). Keep expanding the update rule leads to

\[
\frac{\|V^T F_{t+1}w\|^2}{\|F_{t+1}w\|^2} \geq \frac{\|V^T F_tw\|^2 + 2\eta_t \langle V^T F_tw, V^T AF_tw \rangle}{\|F_tw\|^2 + 2\eta_t \langle F_tw, AF_tw \rangle + B\|F_tw\|^2 \eta_t^2} \tag{55}
\]

\[
= \frac{\|V^T u\|^2 + 2\eta_t \langle V^T u, V^T Au \rangle}{1 + 2\eta_t \langle u, Au \rangle + B\eta_t^2}
\]

\[
\geq \left\{ \|V^T u\|^2 + 2\eta_t \langle V^T u, V^T Au \rangle \right\} \{1 - 2\eta_t \langle u, Au \rangle - B\eta_t^2 \}
\]

\[
\geq \|V^T u\|^2 + 2\eta_t \langle V^T u, V^T Au \rangle - 2\eta_t \|V^T u\|^2 \langle u, Au \rangle - 5\eta_t^2 B^2 - 2\eta_t^3
\]

\[= c^2 + 2\eta_t \{ u^T VV^TAu - c^2 u^TAu \} - \beta_t
\]

\[= c^2 + 2\eta_t u^T(VV^T - c^2 I)Au - \beta_t
\]

\[= c^2 + 2\eta_t u^T(s^2 VV^T - c^2 V_1 V_1^T)Au - \beta_t.
\]

Recall that \( A = V\Lambda_k V^T + V_1 \Lambda_{k+1} V_1^T \). Then

\[
u^T(s^2 VV^T - c^2 V_1 V_1^T)Au = s^2 u^T V\Lambda_k V^T u - c^2 u^T V_1 \Lambda_{k+1} V_1^T u \tag{56}
\]

\[\geq \lambda_k s^2 c^2 - \lambda_{k+1} c^2 s^2 = s^2 c^2 (\lambda_k - \lambda_{k+1})
\]

The recurrence is therefore

\[
\cos^2 \theta (V, F_{t+1}) \geq c^2 + 2\eta_t s^2 c^2 (\lambda_k - \lambda_{k+1}) - \beta_t \tag{57}
\]

\[= c^2 (1 + 2\eta_t (\lambda_k - \lambda_{k+1}) (1 - c^2)) - \beta_t.
\]

The first term is a quadratic function of \( c^2 \):

\[x (1 + a (1 - x)) \tag{58}
\]

where \( x := c^2 \) and \( a = 2\eta_t (\lambda_k - \lambda_{k+1}) \). It has two roots at 0 and \( 1 + \frac{1}{a} \). Therefore, if \( \frac{1}{2} + \frac{1}{2a} \geq 1 \), it is a monotonic increasing function in the interval of \([0, 1]\).

Thus, if \( \eta_t \leq \frac{1}{4(\lambda_k - \lambda_{k+1})} \), which holds for all \( t \) large enough, we have

\[
\cos^2 \theta (V, F_{t+1}) \geq \cos^2 \theta (V, F_t) (1 + 2\eta_t (\lambda_k - \lambda_{k+1}) (1 - \cos^2 \theta (V, F_t))) - \beta_t \tag{59}
\]

which leads to the lemma. \( \square \)

C.1.2 Using different operators in different iterations

Now consider the case of stochastic update rule [43] where we use a mini-batch to approximate the expectation in each iteration.

**Lemma 9.** Let the sequence \( \{F_t\}_t \) be obtained from the update rule [43], then

\[1 - \cos^2 \theta (V, F_{t+1}) \leq [1 - \cos^2 \theta (V, F_t)] [1 - 2\eta_t (\lambda_k - \lambda_{k+1} - \|A_t - A\|) \cos^2 \theta (V, F_{t+1})] + \beta_t,
\]

where \( \beta_t = 5\eta_t^2 B^2 + 3\eta_t^3 B^3 \) and \( \lambda_k \) and \( \lambda_{k+1} \) are the top \( k \) and \( k + 1 \)-th eigenvalues of \( A \).
Proof. The effect of the stochastic update is an additional term in the recurrence
\[
\cos^2 \theta (V, F_{t+1}) \geq c^2 + 2\eta_t u^\top (s^2 V V^\top - c^2 V_1^\top V_1^\top - c^2 V_2^\top V_2^\top) A u + Z_t - \beta_t
\]
where
\[
Z_t = 2\eta_t u^\top (s^2 V V^\top - c^2 V_1^\top V_1^\top) (A_t - A) u.
\]

The effect of the noise can be bounded, i.e.
\[
Z_t = 2\eta_t s^2 u^\top V V^\top (A_t - A) u - 2\eta_t c^2 u^\top V_1^\top V_1^\top (A_t - A) u - 2\eta_t c^2 u^\top (V_1^\top V_1^\top + l_1 I) (A_t - A) u,
\]
where \(s^2 l_1 = c^2 l_2\) are positive numbers such that \(VV^\top + l_1 I\) and \(V_1^\top V_1^\top + l_2 I\) are positive-definite.

The generalized Rayleigh quotient leads to the inequality
\[
|u^\top (VV^\top + l_1 I) (A_t - A) u| \leq \lambda u^\top (VV^\top + l_1 I) u \leq \lambda (c^2 + l_1)
\]
where \(\lambda\) is the largest generalized eigen-value that satisfies
\[
(VV^\top + l_1 I) (A_t - A) x = \lambda (VV^\top + l_1 I) x.
\]
Since \(VV^\top + l_1 I\) is positive definite, we have \(\lambda = \|A_t - A\|\).

Similarly, we have
\[
|u^\top (V_1^\top V_1^\top + l_2 I) (A_t - A) u| \leq \|A_t - A\| (s^2 + l_2).
\]

The noise term is thus bounded by
\[
Z_t \geq -2\eta_t s^2 \|A_t - A\| (c^2 + l_1) - 2\eta_t c^2 \|A_t - A\| (s^2 + l_2).
\]

Note that \(l_1\) and \(l_2\) can be infinitely small positive so we can ignore them.

Therefore, the recurrence is
\[
\cos^2 \theta (V, F_{t+1}) \geq c^2 + 2\eta_t s^2 c^2 (\lambda_k - \lambda_{k+1}) - 4\eta_t \|A_t - A\| s^2 c^2 - \beta_t
\]
\[
= c^2 (1 + 4\eta_t (\lambda_k - \lambda_{k+1} - 2 \|A_t - A\|) (1 - c^2)) - \beta_t
\]

which then leads to the lemma.

In order to get fast convergence, we need to take sufficiently large mini-batches such that the variance of the noise is small enough compared with the eigen-gap.

C.2 Stochastic update without normalization

We show that the cosine angles of the two updates are first-order equivalent. Then, since the recurrence is not affected by higher order terms, when the step size is small enough, we can show it also converges in \(O(1/t)\).

To show the first order equivalence, we need to compare the subspaces obtained by applying the them on the same subspace \(G_t\). So we introduce \(F(G_t)\) to denote the subspace by applying the update rule of \(F_t\) on \(G_t\):
\[
\tilde{F}(G_t) \leftarrow G_t + \eta_t A_t G_t
\]
\[
F(G_t) \leftarrow \tilde{F}(G_t) \left[\tilde{F}(G_t)\top \tilde{F}(G_t)\right]^{-1/2}
\]
Then the first order equivalence as stated in Lemma 4 follows from the following two lemmas for the normalized update rule (43) and the unnormalized update rule (68), respectively.
Lemma 10. \( \cos^2 \theta (V, F(G_t)) = \lambda_{\min} (M + O(\eta^2)) \) where
\[
M = V^T P P^T V + \eta V^T P P^T AV + \eta V^T A P P^T V - 2\eta V^T P P^T A P P^T V,
\]
where \( P P^T = G_t (G_t^T G_t)^{-1} G_t^T \), and \( P \) is an orthonormal basis for the subspace \( G_t \).

Proof. For simplicity, let \( G \) denote \( G_t \), and let \( A \) denote \( A_t \) in the following. We first have
\[
\cos^2 \theta (V, F(G)) = \lambda_{\min} \left( V^T F(G) F(G)^T V \right) = \lambda_{\min} \left( F(G)^T V V^T F(G) \right)
= \lambda_{\min} \left\{ V^T (G + \eta_t A G) \left[ (G + \eta_t A G)^T (G + \eta_t A G) \right]^{-1} (G + \eta_t A G)^T V \right\}.
\]

Note that (70) is due to the fact that
\[
\lambda_{\min} \left( F(G)^T V V^T F(G) \right) = \min_w \frac{w^T F(G)^T V V^T F(G) w}{w^T w}
= \min_z \frac{z^T (G + \eta_t A G)^T V V^T (G + \eta_t A G) z}{z^T R z}
= \min_z \frac{z^T (G + \eta_t A G)^T V V^T (G + \eta_t A G) z}{z^T (G + \eta_t A G)^T (G + \eta_t A G) z}
= \min_z \frac{\|V^T (G + \eta_t A G) z\|^2}{\|(G + \eta_t A G) z\|^2}
\]
where \( R = \left( (G + \eta_t A G)^T (G + \eta_t A G) \right)^{1/2} \).

Now turn back to (71). Expand the matrix-valued function
\[
\phi(\eta) = \left[ (G + \eta_t A G)^T (G + \eta_t A G) \right]^{-1}
= \phi(0) + \phi'(0) \eta + O(\eta^2).
\]

\[
\phi'(0) = -2 \left( (G^T G)^{-1} G^T A G (G^T G)^{-1} \right).
\]

So,
\[
\phi(\eta) = (G^T G)^{-1} - 2 \eta (G^T G)^{-1} G^T A G (G^T G)^{-1} + O(\eta^2).
\]

Therefore,
\[
V^T (G + \eta_t A G) \left[ (G + \eta_t A G)^T (G + \eta_t A G) \right]^{-1} (G + \eta_t A G)^T V
= (V^T G + \eta_t V^T A G) \left[ (G^T G)^{-1} - 2 \eta (G^T G)^{-1} G^T A G (G^T G)^{-1} + O(\eta^2) \right] (G^T V + \eta_t G^T AV)
= V^T G (G^T G)^{-1} G^T V + \eta V^T G (G^T G)^{-1} G^T AV + \eta V^T A G (G^T G)^{-1} G^T V
- 2\eta V^T G (G^T G)^{-1} G^T A G (G^T G)^{-1} G^T V + O(\eta^2)
= V^T P P^T V + \eta V^T P P^T AV + \eta V^T A P P^T V - 2\eta V^T P P^T A P P^T V + O(\eta^2),
\]
where \( P P^T = G (G^T G)^{-1} G^T \), and \( P \) is an orthonormal basis for the subspace \( G \). \(\square\)
Lemma 11. \( \cos^2 \theta(V,G_{t+1}) = \lambda_{\min}(M) \) where \( M \) is as defined in Lemma \[10\].

Proof. For simplicity, let \( G \) denote \( G_t \) and let \( A \) denote \( A_t \). Then \( \cos^2 \theta(V,G_{t+1}) = \lambda_{\min}(N) \), where

\[
N = V^T G_{t+1} \left[ (G_{t+1}^T G_{t+1})^{-1} \right] G_{t+1}^T V \quad \text{with} \quad G_{t+1} = G + \eta (I - GG^T) AG.
\]

Now it suffices to show \( N = M \). Consider

\[
\phi(\eta) = \left[ (G + \eta (I - GG^T) AG) \right] \left[ (G + \eta (I - GG^T) AG) \right]^{-1}.
\]

Then

\[
\phi'(0) = -\left( G^T G \right)^{-1} \left[ G^T (I - GG^T) AG + G^T A (I - GG^T) G \right] \left( G^T G \right)^{-1}
\]

Therefore, \( N \) is

\[
V^T (G + \eta (I - GG^T) AG) \left[ (G + \eta (I - GG^T) AG) \right] \left[ (G + \eta (I - GG^T) AG) \right]^{-1} \times \left( G + \eta (I - GG^T) AG \right)^T V
\]

\[
= \left( V^T G + \eta V^T (I - GG^T) AG \right) \left[ (G + \eta (I - GG^T) AG) \right] \left[ (G + \eta (I - GG^T) AG) \right]^{-1} \times \left( G + \eta (I - GG^T) AG \right)^T V
\]

\[
= \left( V^T G + \eta V^T (I - GG^T) AG \right) \times \left[ (G^T G)^{-1} - \eta (G^T G)^{-1} \left[ G^T (I - GG^T) AG + G^T A (I - GG^T) G \right] (G^T G)^{-1} \right] \times \left( G + \eta (I - GG^T) AG \right)^T V
\]

\[
= V^T G (G^T G)^{-1} G^T V + \eta V^T G (G^T G)^{-1} G^T A (I - GG^T) V + \eta V^T (I - GG^T) AG (G^T G)^{-1} G^T V
\]

which completes the proof. \( \square \)

D Doubly Stochastic Update

In this section, we consider the doubly stochastic update rule. Suppose in step \( t \), we use a mini-batch consisting of \( B_{x,t} \) random data points \( x_i^t (1 \leq i \leq B_{x,t}) \) and \( B_{\omega,t} \) random features \( \omega_j^t (1 \leq j \leq B_{\omega,t}) \). Then the update rule is

\[
H_{t+1} = H_t + \eta \mathbb{E}_t [\phi_{\omega_i}(x_i)h_i(x_i)] - \eta \mathbb{E}_t [h_i^T(x_i)h_i(x_i)]
\]  \hspace{1cm} (76)

\[
H_t = H_t (I - \eta \mathbb{E}_t [h_i(x_i)] - \eta \mathbb{E}_t [\phi_{\omega_i}(x_i)])
\]  \hspace{1cm} (77)

where for any function \( f(x,\omega) \), \( \mathbb{E}_t f(x_i,\omega) \) denotes \( \sum_{i=1}^{B_{x,t}} \sum_{j=1}^{B_{\omega,t}} f(x_i^i,\omega_j^i)/(B_{x,t}B_{\omega,t}) \). As before, we assume \( H_0 = F_0 \) is a good initialization, i.e., \( F_0^T F_0 = I \) and \( \cos^2 \theta(F_0,V) \geq 1/2 \). Note that \( H_t = [h_1^T(\cdot),\ldots,h_t^T(\cdot)] \), while \( h_i(x_i) \) is its evaluation at \( x_i \), i.e., \( h_i(x_i) \) is a row vector \( [h_i^T(x_i),\ldots,h_i^T(x_i)] \).
We introduce the following intermediate function for analysis:

\[
\tilde{G}_{t+1} = \tilde{G}_t + \eta_t E_t [k(x_t, \cdot) h_t(x_t)] - \eta_t \tilde{G}_t E_t [h_t(x_t) \top h_t(x_t)]
\]

(78)

\[
= \tilde{G}_t (I - \eta_t E_t [h_t(x_t) \top h_t(x_t)]) + \eta_t E_t [k(x_t, \cdot) h_t(x_t)]
\]

(79)

Again, \(\tilde{G}_0 = F_0\).

The analysis follows our intuition: we first bound the difference between \(H_t\) and \(\tilde{G}_t\) by a martingale argument, and then bound the difference between \(\tilde{G}_t\) and \(V\). For the second step we can apply the previous argument. Note that \(G_t\) is different from \(F_t\) since \(A_t F_t = k(x,t,\cdot) F_t(x_t)\) is now replaced by \(k(x_t,\cdot) h_t(x_t)\), so we need to adjust our previous analysis.

Suppose we use random Fourier features for points in \(\mathbb{R}^d\), see [23]. Then we have

**Theorem 5.** Suppose the mini-batch sizes satisfy that for any \(1 \leq i \leq t\), \(\|A_t - A_i\| < (\lambda_k - \lambda_{k+1})/8\) and \(B_{x,i} = O(\ln \frac{t}{\delta})\). There exist \(B_{\omega,i} = O(\ln \frac{t}{\delta})\) and step sizes \(\eta_i = O(1/i)\), such that the following holds. If \(\Omega(1) = \lambda_k(G_t^\top G_t) \leq \lambda_1(\tilde{G}_t^\top \tilde{G}_t) = O(1)\) for all \(1 \leq i \leq t\), then for any \(x\) and any function \(v\) in the span of \(V\) with unit norm \(\|v\|_F = 1\), we have that with probability \(1 - \delta\), there exists \(h\) in the span of \(H_t\) satisfying

\[
|v(x) - h(x)|^2 = O \left( \frac{1}{t} \ln \frac{t}{\delta} \right).
\]

Proof. Let \(w = \tilde{G}_t^\top v\), \(\tilde{g} = \tilde{G}_t w\), and \(h = H_t w\).

\[
|v(x) - h(x)|^2 = |v(x) - \tilde{g}(x) + \tilde{g}(x) - h(x)|^2
\]

\[
\leq 2 |v(x) - \tilde{g}(x)|^2 + 2 |\tilde{g}(x) - h(x)|^2
\]

\[
\leq 2 \|v - \tilde{g}\|_F^2 \|k(x, \cdot)\|_F^2 + 2 |\tilde{g}(x) - h(x)|^2
\]

\[
\leq 2 \kappa^2 \|v - \tilde{g}\|_F^2 + |\tilde{g}(x) - h(x)|^2.
\]

Roughly speaking, the difference between \(v\) and \(\tilde{g}\) is the error due to random data points and can be bounded by Lemma 13, while the difference between \(\tilde{g}(x)\) and \(h(x)\) is the error due to random features and can be bounded by Lemma 13. More precisely, since \(\tilde{g}\) is the projection of \(v\) on the span of \(\tilde{G}_t\),

\[
\|v - \tilde{g}\|_F^2 = \|v\|_F^2 - \|\tilde{g}\|_F^2 \leq 1 - \cos^2 \theta(\tilde{G}_t, V) = O \left( \frac{1}{t} \ln \frac{t}{\delta} \right)
\]

where the last step is by Lemma 15. Also, since \(\|w\| = 1\), we have \(|\tilde{g}(x) - h(x)|^2 = O \left( \frac{1}{t} \ln \frac{t}{\delta} \right)\) by Lemma 13.

What is left is to check the mini-batch sizes; see the assumptions in Lemma 12 and Lemma 15. We need \(\lambda_k(E_t [h_t(x_t) \top h_t(x_t)]) = \lambda_k(E_x [h_t(x) \top h_t(x)]) + O(1)\), so we only need to estimate \(E_x [h_t(x) \top h_t(x)]\) up to constant accuracy for all \(1 \leq j, \ell \leq k\), for which \(B_{x,i} = O(\ln \frac{t}{\delta})\) suffices. We also need \(\Delta_\omega = O(\lambda_k - \lambda_{k+1}) = O(1)\), so we only need \(\Delta_\omega = O(1)\). This is a bound for \((tB_{x,i})^2\) pairs of points, for which \(B_{\omega,i} = O(\ln \frac{t}{\delta})\) suffices.

Similar bounds hold for other random features, where the batch sizes will depend on the concentration bound of the random features used.

The rest of this section is the proof of the theorem. For simplicity, \(\|\cdot\|_F\) is shorten as \(\|\cdot\|\).

First, we bound the difference between \(H_t\) and \(\tilde{G}_t\).

**Lemma 12.** Suppose \(|k(x, x')| \leq \kappa, |\phi(x)| \leq \phi\). For any \(w\) and \(x\), with probability \(1 - \delta\) over \((D^t, \omega^t)\),

\[
|\tilde{g}_{t+1}(x) w - h_{t+1}(x) w|^2 \leq B_{t+1}^2 := \frac{1}{2} (\kappa + \phi)^2 \ln \left( \frac{2}{\delta} \sum_{i=1}^t |E_t |h_t(x_i)| a_{t,i} w|^2 \right)
\]

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where \( a_{t,i} = \eta_t \prod_{j=i+1}^t (I - \eta_j \mathbb{E}_j [h_j(x_j)^\top h_j(x_j)]) \) for \( 1 \leq i \leq t \), and \( |h_i(x_i)| := \left[ \left| h_i^j(x_i) \right| \right]_{j=1}^k \).

Furthermore, for any \( x \) and \( w \),

\[
\mathbb{E}_{D_t^i, \omega_i} |\tilde{g}_{t+1}(x) - h_{t+1}(x)|^2 \leq B_{2,t+1}^2 := (\kappa + \phi)^2 \sum_{i=1}^t |\mathbb{E}_i |h_i(x_i)| a_{t,i}w|^2.
\]

Suppose the mini-batch sizes are large enough so that \( |k(x_i, x_i') - \sum_{j=1}^{B_{\omega,i}} \phi_{\omega_i}(x_i') \phi_{\omega_i}(x_i')/B_{\omega,i}| \leq \Delta_\omega \) for all sampled data points \( x_i \) and \( x_i' \). Then the two bounds hold for any \( x \) in the sampled point set with \( (\kappa + \phi)^2 \) replaced by \( \Delta_\omega^2 \).

Proof. Note that

\[
H_{t+1} = \sum_{i=1}^t \mathbb{E}_i [\phi_{\omega_i}(x_i) \phi_{\omega_i}(x_i) h_i(x_i)] a_{t,i} + F_0 a_{t,0},
\]

and

\[
\tilde{G}_{t+1} = \sum_{i=1}^t \mathbb{E}_i [k(x_i, x_i') h_i(x_i)] a_{t,i} + F_0 a_{t,0},
\]

where \( a_{t,0} = \prod_{j=1}^t (I - \eta_j \mathbb{E}_j [h_j(x_j)^\top h_j(x_j)]) \).

We have \( \tilde{g}_{t+1}(x) - h_{t+1}(x) = \sum_{i=1}^t V_{t,i}(x) \) where

\[
V_{t,i}(x) = \mathbb{E}_i [k(x_i, x) h_i(x_i) - \phi_{\omega_i}(x_i) \phi_{\omega_i}(x_i) h_i(x_i)] a_{t,i}w.
\]

This \( V_{t,i}(x) \) is a function of \( (D_i^i, \omega^i) \) and

\[
\mathbb{E}_{D_t^i, \omega_i} [V_{t,i}(x)|\omega^{i-1}] = \mathbb{E}_{D_t^i, \omega_i} [V_{t,i}(x)|\omega^{i-1}] = 0,
\]

so \( \{V_{t,i}(x)\} \) is a martingale difference sequence. Since \( |V_{t,i}(x)| < (\kappa + \phi) |\mathbb{E}_i |h_i(x_i)| a_{t,i}w| \), the first two statements follow from Azuma’s Inequality. When \( x \) is a sampled point, \( |V_{t,i}(x)| < \Delta_\omega |\mathbb{E}_i |h_i(x_i)| a_{t,i}w| \), the final part of the lemma follows.

So to bound \( |\tilde{g}_t(x)w - h_t(x)w| \), we need to bound \( |\mathbb{E}_i |h_i(x_i)| a_{t,i}w| \), which requires some additional assumptions.

Lemma 13 (Complete version of Lemma 7). Suppose the conditions in Lemma 13 are true. Further suppose for all \( i \leq t \), \( \eta_i = \theta/i \) where \( \theta \) is sufficiently large so that \( \theta \lambda_k(\mathbb{E}_i [h_i(x_i)^\top h_i(x_i)]) \geq 1 \); also suppose \( \lambda_1 \left( \tilde{G}_i^\top \tilde{G}_i \right) = O(1) \).

(1) With probability \( \geq 1 - \delta \) over \( (D^t, \omega^t) \), for all \( 1 \leq i \leq t \) and \( \ell \in [k] \), we have

\[
|\tilde{g}_i^\ell(x_i) - h_i^\ell(x_i)|^2 = O \left( \frac{\Delta^2 \theta^4}{t} \ln \left( \frac{t}{\delta} \right) \right).
\]

(2) For any \( x \) and unit vector \( w \), with probability \( \geq 1 - \delta \) over \( (D^t, \omega^t) \),

\[
|\tilde{g}_t(x)w - h_t(x)w|^2 = O \left( \frac{\theta^4}{t} \ln \left( \frac{t}{\delta} \right) \right).
\]

(3) For any \( x \) and unit vector \( w \),

\[
\mathbb{E}_{D_t^i, \omega_i} |\tilde{g}_t(x)w - h_t(x)w|^2 = O \left( \frac{\theta \ln t}{t} \right).
\]
Proof. We first do induction on statement (1), which is true initially. Assume it is true for \( t \), we prove it for \( t + 1 \).

We have that for any unit vector \( w \),

\[
|E_i | h_i(x_i) | a_{t,i} w | = \left| \eta_i E_i | h_i(x_i) | \prod_{j=i+1}^{t} \left[ I - \eta_j E_j \left[ h_j(x_j)^T h_j(x_j) \right] \right] w \right| \]

\[
\leq \eta_i \| E_i | h_i(x_i) \| \| w \| \prod_{j=i+1}^{t} \| I - \eta_j E_j \left[ h_j(x_j)^T h_j(x_j) \right] \| \\
\leq O(1) \frac{\theta^2}{t} \prod_{j=i+1}^{t} \left( 1 - \frac{1}{j} \right) = O \left( \frac{\theta^2}{t} \right).
\]

We use in the second line

\[
\| h_i(x_i) \| \leq O \left( \sqrt{\frac{\theta^2}{t} \ln \frac{t}{\delta}} \right) + \| g_i(x_i) \| \leq O \left( \sqrt{\frac{\theta^2}{t} \ln \frac{t}{\delta}} \right) + \sqrt{\| G_i^T \hat{G}_i \| \phi(x_i) } = O(\theta)
\]

that holds with probability \( 1 - t\delta/(t+1) \) by induction, and we use in the last line \( \theta \lambda_k \left( E_i \left[ h_i(x_i)^T h_i(x_i) \right] \right) \geq 1 \).

Then by Lemma 13 with probability \( \geq 1 - \delta/(k(t+1)) \),

\[
|\tilde{g}_{t+1}(x_{t+1}) w - h_{t+1}(x_{t+1}) w |^2 \leq \frac{1}{2} \Delta^2 \omega \ln \left( \frac{2(t+1)}{\delta} \right) \sum_{i=1}^{t} |a_{t,i} w|^2 \\
\leq O(\Delta^2 \omega) \ln \left( \frac{t+1}{\delta} \right) \sum_{i=1}^{t} \frac{\Delta^2 \eta^4}{t^2} = O \left( \frac{\theta^4}{t+1} \ln \left( \frac{t+1}{\delta} \right) \right).
\]

Repeating the argument for \( k \) basis vectors \( w = e_i (1 \leq i \leq k) \) completes the proof.

The statements (2)(3) follow from similar arguments. \( \square \)

Next, we bound the difference between \( \tilde{G}_t \) and \( V \).

**Lemma 14.** Suppose the conditions in Lemma 13 are true and furthermore, \( \lambda_k (\tilde{G}_t^T \tilde{G}_t) = \Omega(1) \) for all \( i \in [t] \).

Let \( c^2_t \) denote \( \cos^2 \theta(\tilde{G}_t, V) \). Then with probability \( \geq 1 - \delta \),

\[
c^2_{t+1} \geq c^2_t \left\{ 1 + 2 \eta_t \left[ \lambda_k - \lambda_{k+1} - 2 \| A_t - A \| - O \left( \Delta^2 \omega^2 \frac{1}{t} \ln \frac{t}{\delta} \right) \right] (1 - c^2_t) - O \left( \eta_t \Delta^2 \omega^2 \frac{1 - c^2_t}{t} \ln \frac{t}{\delta} \right) \right\} - \beta_t
\]

where \( \beta_t \) is as defined in Lemma 3.

**Proof.** The potential of \( \tilde{G}_t \) can be computed by a similar argument as in the previous section; the only difference is replacing \( A_t u \) with \( k(x_t, \cdot) h_t(x_t) \tilde{w} \). This leads to

\[
\cos^2 \theta(\tilde{G}_{t+1}, V) \geq c^2 + 2 \eta_t u^T \left( s^2 V V^T - c^2 V_{\perp} V_{\perp}^T \right) k(x_t, \cdot) h_t(x_t) \tilde{w} - \beta_t \\
= c^2 + 2 \eta_t u^T \left( s^2 V V^T - c^2 V_{\perp} V_{\perp}^T \right) \left[ (k(x_t, \cdot) h_t(x_t) \tilde{w} - A_t u) + (A_t u - A_t u) + A_t u - \beta_t \right)
\]

where \( u = \tilde{G}_t \tilde{w} \) with unit norm \( \| u \| = 1 \).

The terms involving \( (A_t u - A_t u) \) and \( A_t u \) can be dealt with as before, so we only need to bound the extra term

\[
u^T \left( s^2 V V^T - c^2 V_{\perp} V_{\perp}^T \right) \left[ k(x_t, \cdot) h_t(x_t) \tilde{w} - A_t u \right] \\
= u^T \left( s^2 V V^T - c^2 V_{\perp} V_{\perp}^T \right) \left[ k(x_t, \cdot) h_t(x_t) \tilde{w} - k(x_t, \cdot) \tilde{g}_t(x_t) \tilde{w} \right] \\
= u^T \left( s^2 V V^T - c^2 V_{\perp} V_{\perp}^T \right) k(x_t, \cdot) [h_t(x_t) - \tilde{g}_t(x_t)] \tilde{w}.
\]
So we need to bound $|h_t(x_t) - \tilde{g}_t(x_t)|\tilde{w}$, which in turn relies on Lemma 13. More precisely, we have $\|h_t(x_t) - \tilde{g}_t(x_t)\|_\infty \leq \hat{O}\left(\Delta_\omega \theta^2 \sqrt{1/t}\right)$ with probability $\geq 1 - \delta$. Also, we have $u = \tilde{G}_t\tilde{w}$ has unit norm, so $\|\tilde{w}\| = O(1)$ when $\lambda_k(\tilde{G}_t^\top \tilde{G}_t) = \Omega(1)$. Then

$$
|u^T V V^T k(x_t, \cdot)h_t(x_t) - \|k(x_t, \cdot)\| \hat{O}\left(\Delta_\omega \theta^2 \sqrt{1/t}\right) \leq c^2 \hat{O}\left(\Delta_\omega \theta^2 \sqrt{1/t}\right)
$$

where the last step follows from $c \geq 1/2$ by assumption. Similarly,

$$
|u^T V \perp V^T k(x_t, \cdot)h_t(x_t) - \|k(x_t, \cdot)\| \hat{O}\left(\Delta_\omega \theta^2 \sqrt{1/t}\right) \leq s\hat{O}\left(\Delta_\omega \theta^2 \sqrt{1/t}\right) = \hat{O}\left(\Delta_\omega \theta^2 \sqrt{\frac{1-c^2}{t}}\right).
$$

Plugging into (82) and apply a similar argument as in Lemma 8 and 9 we have the lemma.

\[ \]

Lemma 15 (Complete version of Lemma 6). If the mini-batch sizes are large enough so that $\|A - A_t\| < (\lambda_k - \lambda_{k+1})/8$, $\lambda_k(\mathbb{E}_i [h_t(x_t)\perp h_i(x_i)]) = \lambda_k(\mathbb{E}_x [h_t(x)\perp h_i(x)]) \pm O(1)$, and $\Delta_\omega = O(\lambda_k - \lambda_{k+1})$, then

1. $\theta = O(1)$;
2. $1 - c^2_t = O\left(\frac{1}{t} \ln \frac{1}{\delta}\right)$.

Proof: If the mini-batch size is large enough so that $\lambda_k(\mathbb{E}_i [h_t(x_t)\perp h_i(x_i)]) = \lambda_k(\mathbb{E}_x [h_t(x)\perp h_i(x)]) \pm O(1)$, we only need to show $\lambda_k(\mathbb{E}_x [h_t(x)\perp h_i(x)]) = \Omega(1)$, which will lead to $\theta = O(1)$ and then solving the recurrence in Lemma 14 leads to $1 - \cos^2(\theta \tilde{G}_t, V) = \hat{O}(1/t)$.

Let $e_i(x) = h_t(x) - \tilde{g}_t(x)$. Then

$$
\mathbb{E}_x [h_t(x)\perp h_i(x)] = \mathbb{E}_x [\tilde{g}_t(x)\perp \tilde{g}_i(x)] + 2\mathbb{E}_x [e_i(x)\perp h_i(x)] - \mathbb{E}_x [e_i(x)\perp e_i(x)].
$$

By Lemma 13, $\mathbb{E}_x [e_i(x)] = \hat{O}(\theta^4/t)$, which is $o(1)$ if $\theta = O(1)$. Then the norm of $2\mathbb{E}_x [e_i(x)\perp h_i(x)] - \mathbb{E}_x [e_i(x)\perp e_i(x)]$ is $o(1)$, so we only need to consider $\mathbb{E}_x [\tilde{g}_t(x)\perp \tilde{g}_i(x)]$.

Formally, we prove our statements (1)(2) by induction. For this reason, view $\theta$ as

$$
\theta = 1/\min_{1 \leq i \leq t} \lambda_k(\mathbb{E}_i [h_t(x)\perp h_i(x)]).
$$

They are true initially. Suppose they are true for $t - 1$, we prove them for $t$.

First, by solving the recurrence for $c_t$, we have that statement (2) is true up to step $t$.

Next, since $\mathbb{E}_x [\tilde{g}_t(x)^\top \tilde{g}_i(x)] = \tilde{G}_t^\top A \tilde{G}_i$, we have

$$
w^\top \mathbb{E}_x [\tilde{g}_t(x)^\top \tilde{g}_i(x)] w = w^\top \tilde{G}_t^\top A \tilde{G}_i w
= w^\top \tilde{G}_t^\top (V \Lambda_k V^\top + V_{\perp} A_{\perp} V_{\perp}^\top) \tilde{G}_i w
\geq w^\top \tilde{G}_t^\top V \Lambda_k V^\top \tilde{G}_i w
\geq \lambda_k w^\top c_t^2 \| \tilde{G}_i w \|
$$

which means $\lambda_k(\mathbb{E}_x [\tilde{g}_t(x)^\top \tilde{g}_i(x)]) = \Omega(1)$ by induction on $c_t$ and by the assumption that $\lambda_k(\tilde{G}_t^\top \tilde{G}_i) = \Omega(1)$. This then leads to $\lambda_k(\mathbb{E}_i [h_t(x)\perp h_i(x)]) = \Omega(1)$, which means $\theta = O(1)$ up to step $t$. \[ \]