Achieving Statistical Optimality of Federated Learning: Beyond Stationary Points

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Abstract

Federated Learning (FL) is a promising framework that has great potentials in privacy preservation and in lowering the computation load at the cloud. FedAvg and FedProx are two widely adopted algorithms. However, recent work raised concerns on these two methods: (1) their fixed points do not correspond to the stationary points of the original optimization problem, and (2) the common model found might not generalize well locally.

In this paper, we alleviate these concerns. Towards this, we adopt the statistical learning perspective yet allow the distributions to be heterogeneous and the local data to be unbalanced. We show, in the general kernel regression setting, that both FedAvg and FedProx converge to the minimax-optimal error rates. Moreover, when the kernel function has a finite rank, the convergence is exponentially fast. Our results further analytically quantify the impact of the model heterogeneity and characterize the federation gain – the reduction of the estimation error for a worker to join the federated learning compared to the best local estimator. To the best of our knowledge, we are the first to show the achievability of minimax error rates under FedAvg and FedProx, and the first to characterize the gains in joining FL. Numerical experiments further corroborate our theoretical findings on the statistical optimality of FedAvg and FedProx and the federation gains.

1 Introduction

Federated Learning (FL) is a rapidly developing learning framework in which a parameter server (PS) coordinates with a massive collection of end devices in executing machine learning tasks \cite{KMY+16, KMRR16, MMR+17, KMA+19}. In FL, instead of uploading data to the PS, the end devices work at the front line in processing their own local data and periodically report their local updates to the PS. The PS then effectively aggregates those updates to obtain a fine-grained model and broadcasts the fine-grained model to the end devices for further model updates. On the one hand, FL has great potentials in privacy-preservation and in lowering the computation load at the cloud, both of which are crucial for modern machine learning applications. On the other hand, costly communication, massively-distributed system architectures, and highly unbalanced and heterogeneous data across devices are among the defining challenges of FL.

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FedAvg and FedProx are two widely adopted FL algorithms [MMR+17, LSZ+18]. Under FedAvg, to save communication, the local updates are only aggregated after every $s$-th local steps, where $s \geq 1$; when $s = 1$, FedAvg reduces to the standard SGD algorithm. FedProx is a proximal-variant of FedAvg and is used to better tolerate the heterogeneity in FL. Despite ample recent effort and some progress, understandings of these two methods, especially of FedAvg, remain elusive [KMA+19]. What’s worse, several recent work independently pointed out that FedAvg with $s \geq 2$ and FedProx fail to minimize the global objective even in the simplest homogeneous setting [PW20, KKM+20, ZLL+18]. Besides, under FedAvg and FedProx, only a common model is trained but is used to serve all the participating end devices, which could be problematic in the presence of heterogeneity [FMO20, DKM20, DTN20].

Driven by these pessimistic findings, recent work starts abandoning FedAvg and FedProx and proposes new algorithms [PW20, KKM+20, FMO20, DKM20, DTN20].

In this paper, we make progresses in deepening the understandings of FedAvg and FedProx by alleviating the concerns on their unreachability to stationary points and lack of model personalization. Specifically, two of the key messages are:

(M.1) Unreachability to stationary points does not prevent successful learning.

(M.2) Individual end devices still benefit from FL despite lack of model personalization.

On (M.1): Most work on the convergence of FedAvg and FedProx centers around minimizing

$$L(\theta) = \sum_{i=1}^{M} L_i(\theta)$$

– the centralized empirical risk function – where $L_i(\theta)$ is the local empirical risk each worker assigned to the model parameter $\theta$ [KMA+19, MMR+17, LSZ+18, KKM+20]. The focus is on analyzing whether or not the stationary points of $L(\theta)$ can be achieved. Recent seminal work [KKM+20, ZLL+18, PW20] showed, both experimentally and theoretically, that FedAvg fails to minimize (1) even in the data homogeneous setting except for the special case when $s = 1$. This observation is also illustrated in Fig.1a, wherein we plot the trajectories of the gradient magnitudes $\|\nabla L(\theta_t)\|_2$ versus the communication rounds $t$ under FedProx and FedAvg with aggregation period $s$ being 1, 5, 10, respectively. While the gradient magnitude of FedAvg with $s = 1$ quickly drops to 0, the gradient magnitudes under FedProx and FedAvg with $s = 5, 10$ stay well above 0. A natural yet fundamental question arises: Does the failure of reaching stationary points lead to unsuccessful learning? In this paper, we answer this question in the negative by exploring beyond the stationary points. We show that both FedAvg and FedProx can achieve the minimax-optimal estimation error. In particular, as illustrated in Fig.1b, both FedAvg with $s = 5, 10$ and FedProx quickly converge to almost the same low estimation error as FedAvg with $s = 1$. Moreover, the convergence time of FedAvg with $s = 5, 10$ shrinks roughly by a factor of $s$ compared to $s = 1$.

On (M.2): Little attention has been paid to analytically characterizing the gains and losses for an end device owner to participate in FL. In FL, a common model is trained to serve the participating end devices. Due to heterogeneity, an end device might not always benefit from its participation. Recent work starts paying attention to model personalization [FMO20, DKM20, DTN20]. In this paper, we take a complementary angle and show that even if only a common model can be obtained, an end device can still gain substantially from participating FL under mild conditions. We rigorously characterize such conditions. Towards this end, we introduce the notion of federation gain, defined as the ratio between the lowest achievable error of a model trained on local data and the estimation error of a model trained via FL; see Section 4.4 for a formal definition.
Our contributions: Formally, our results can be summarized as follows. We show that both FedAvg and FedProx can achieve the minimax-optimal estimation error despite the failure of the convergence to the stationary points of the global empirical risk function. Our analysis allows the data distributions and local models to be heterogeneous and accommodates highly unbalanced data partition across end devices. More specifically, we show, in the non-parametric regression setting, that

- On prediction errors: Both FedAvg and FedProx achieve low errors for both in-sample and out-sample (generalization) prediction. Our results apply to the general setting where the underlying truth function belongs to a reproducing kernel Hilbert space and yield the minimax optimal rate in specific kernel classes even compared to the best centralized learning algorithms. Our results further characterize the $O(1/t)$ convergence rate in this general setting and show that FedAvg with an appropriately chosen step size can speed up the convergence by a factor of $s$ while enjoying the nearly-optimal final prediction errors.

- On underlying truth recovery: When the kernel function has a finite rank, both FedAvg and FedProx can further learn the underlying model parameter and converge exponentially fast to a minimax-optimal error rate. Our results further quantify the impacts of the model heterogeneity and covariate heterogeneity. We also characterize the federation gain – the reduction of the estimation error for a worker to join the federated learning compared to the best local estimator. Such characterization could be used as a guidance in encouraging end devices owners to make their participation decisions.

- On the technical front: We derive compact matrix form expressions for the recursive dynamics of the global model. A key challenge is that the local update may be far from the previous global model and depends on the local data. The previous studies of FedAvg and FedProx \cite{ZWSL10, Sti18, KKM+20, LSZ+18} focus on simplifying the dynamics. Unfortunately, the simplified dynamics fail to capture the intricate interplay between the local gradient updates and the global averaging step. Towards our matrix form expressions, we derive and crucially employ several novel and delicate block matrix identities that enable us to capture the perturbation of
local updates (See Lemma 1). These identities could be of independent interest in analyzing the first-order iterates.

1.1 Related work

On convergence of FedAvg and FedProx. FedAvg has emerged as the algorithm of choice for FL [KMA+19, KKM+20]. Both empirical success and failures of convergence have been reported [MMR+17, LSZ+18, KKM+20], and the theoretic characterization of its convergence (for general s) turns out to be notoriously difficult. In the absence of data heterogeneity, convergence is shown [ZWSL10, Sti18] under the name local SGD. In particular, [ZWSL10] proved asymptotic convergence. Convergence in the non-asymptotic region was derived in [Sti18] under strong convexity and bounded gradient assumptions. The proof techniques of [ZWSL10, Sti18] were adapted to data heterogeneity setting [KKM+20] under bounded gradient variance and/or uniform bounded gradient or Hessian dissimilarity [KKM+20]. Even stronger assumptions are adopted for the convergence proof of FedProx [LSZ+18]. Most of these results are derived in the context of optimization and focus on the in-sample prediction errors only. Other work assumes fresh data in each update for technical convenience [KMA+19]. Both the randomness in the design matrix, which is harder to handle, and the impacts of the covariate dimension are mostly neglected. In particular, when the randomness in the design matrix is taken into account, ensuring uniform bounded dissimilarity requires the local data size to be much larger than the model dimension – excluding their applicability to locally data scarce applications such as IoT and mobile healthcare.

Personalization. In the context of Model Agnostic Meta Learning (MAML), personalized Federated Learning was investigated both experimentally [CLD+18, JKRK19] and theoretically [FMO20, LYZ20]. MAML-type personalized FL finds an initial shared model that a participating device can quickly get personalized by running a few updates on its local data. Adaptive Personalized Federated Learning (APFL) was proposed in [DKM20] under which each end device trains its local model while contributing to the global model. A personalized model is then learned as a mixture of optimal local and global models. Other personalization techniques include model division, contextualization, and multi-task learning. Due to space limitation, readers are referred to [KMA+19] for details. In this paper, we show that without introducing additional personalization techniques, an end device can still benefit from joining FL under certain mild conditions.

2 Problem Setup

A federated learning system consists of a parameter server (PS) and M workers. Each worker \(i \in \{1, \cdots, M\} = [M]\) locally keeps its personal data \(S_i = \{(x_{ij}, y_{ij})\}_{j=1}^{n_i}\). The volume of the local dataset \(S_i\) varies with different real-world applications. For example, when \(S_i\) are records of recently browsed websites, the volume of \(S_i\) is typically moderate – based on which a reasonably fair but not high-quality model can be trained. When \(S_i\) are records of recent places visited by walk in pandemic, the volume of \(S_i\) is low. We consider synchronous systems, i.e., the computation and communication delays are bounded and known; we will explore the impacts of system asynchrony in our future work.

Our model captures both covariate heterogeneity (a.k.a. covariate shift) and response heterogeneity (a.k.a. concept shift). Specifically, at each worker \(i\), the response \(y_{ij}\) is determined as

\[
y_{ij} = f_i^*(x_{ij}) + \xi_{ij}, \quad 1 \leq j \leq n_i,
\]

where \(f_i^*\) is the underlying mechanism governing the true responses, \(x_{ij} \in \mathcal{X}\) is the covariate, and \(\xi_{ij}\) is the observation noise that is independent across workers. We impose a mild assumption that
\( \eta_i, \cdots, \xi_{in_i} \) are independent (possibly non-identically distributed), zero-mean, and have constant variance up to \( \sigma^2 \). We will consider both the fixed design setting where \( x_{ij} \) is deterministic and random design setting where \( x_{ij} \sim D_i \).

We base our analysis on the standard non-parametric regression setup and assume that \( f_i^* \) belongs to a reproducing kernel Hilbert spaces (RKHS) with a defining kernel function \( k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \). We impose the following minimal assumptions that are common in literature \cite{Wai19}: \( \mathcal{X} \) is compact, \( \sup_{x \in \mathcal{X}} k(x, x) < \infty \), and \( \int_{\mathcal{X} \times \mathcal{X}} k^2(x, y) d\mathbb{P}(x) d\mathbb{P}(y) < \infty \). Mercer’s theorem guarantees that there exists a feature map \( \phi : \mathcal{X} \rightarrow \ell^2(\mathbb{N}) \) such that \( k(x, y) = \langle \phi(x), \phi(y) \rangle \) where \( \ell^2(\mathbb{N}) \) denotes the space of square-summable sequences. Consequently, any \( f \in \mathcal{H} \) can be expressed as \( f(x) = \langle \phi(x), \theta \rangle \) for some \( \theta \in \ell^2(\mathbb{N}) \) and \( \|f\|_{\mathcal{H}} = \|\theta\|_2 \). In particular, \( f_i^*(x) = \langle \phi(x), \theta_i^* \rangle \). Without loss of generality, after proper scaling we assume that \( \|f\|_{\mathcal{H}} \leq 1 \) for all \( f \in \mathcal{H} \). For convenience, we collect a few preliminaries on RKHS in Appendix C.

### 2.1 FedAvg and FedProx

**FedAvg** can be viewed as a communication-light implementation of the standard centralized SGD. Different from the standard SGD, wherein the local updates are aggregated right after every local step, in **FedAvg** the local updates are only aggregated after every \( s \)-th local step, where \( s \geq 1 \) is an algorithm parameter. **FedProx** is a distributed proximal algorithm wherein a round-varying proximal term is introduced to control the deviation of the local updates from the most recent global model.

Detailed implementations of these two algorithms, described in Appendix A, involve many tuning parameters. To make the discuss concrete, we focus on the backbones of **FedAvg** and **FedProx** only. The insights obtained can be adapted for the general implementation.

For ease of exposition, let \( L_t(f) = \frac{1}{2} \sum_{i=1}^{n_i} (f(x_{ij}) - y_{ij})^2 \) denote the local empirical risk function for each \( f \in \mathcal{H} \). Let \( f_t \) denote the global model at the end of the \( t \)-th communication round, and let \( f_0 \) denote the initial global model. At the beginning of each round \( t \geq 1 \), the PS broadcasts \( f_{t-1} \) to each of the \( M \) workers. At the end of round \( t \), upon receiving the local updates \( f_i^t \) from each worker \( i \), the PS updates the global model as \( f_t = \sum_{i=1}^{M} w_i f_i^t \), where \( w_i = \frac{n_i}{N} \) – recalling that \( N \) is the number of all the data tuples in the FL system. The local updates \( f_i^t \) under **FedAvg** and **FedProx** are obtained as follows.

**FedAvg** From \( f_{t-1} \) each worker \( i \) runs \( s \) local gradient descent steps on \( L_t(f) \), and reports its updated model to the PS. Concretely, we denote the mapping of one-step local gradient descent by \( P_t(f) = f - \eta_t \nabla L_t(f) \), where \( \eta_t > 0 \) is the stepsize chosen by worker \( i \) \cite{PW20}. After \( s \) local steps, the locally updated model at worker \( i \) is given by

\[
 f_i^t = P_i^s(f_{t-1}).
\]

**FedProx** From \( f_{t-1} \), each worker \( i \) locally updates the model as

\[
f_i^t = \arg\min_{f \in \mathcal{H}} L_i(f) + \frac{1}{2\eta_i} \|f - f_i^t\|_{\mathcal{H}}^2,
\]

where \( \eta_i > 0 \) controls the regularization and can be interpreted as a step size: As \( \eta_i \) increases, the penalty for moving away from \( f_t \) decreases and hence the local update \( f_i^t \) will be farther way from \( f_t \). Notably, in practice, the local optimization problem in (2) might not be solved exactly in each round. We would like to study the impacts of inexactness of solving (2) in future work.
**Notation** Let \( X_i \) denote the local data matrix whose \( j \)-th row is \( x_{ij} \) and \( X \) denote the global data matrix which stacks \( \{ X_i, i \in [M] \} \) in rows. Similarly, let \( y_i \in \mathbb{R}^{n_i} \) be the column vector that stacks \( y_{ij} \) for \( j = 1, \ldots, n_i \) and \( y = [y_1^\top, \ldots, y_M^\top]^\top \). Denote \( \phi(X_i) : \ell^2(N) \to \mathbb{R}^{n_i} \) as the linear operator such that \( \phi(X_i) = [\phi(x_{i1}), \ldots, \phi(x_{in_i})]^\top \) and \( \phi(X) = [\phi^\top(X_1), \ldots, \phi^\top(X_M)]^\top \). Let \( \|v\|_2 \) and \( \|V\|_2 \) denote the \( \ell^2 \) norm of a vector \( v \) and the spectral norm of matrix \( V \), respectively. For function \( f \in L^2(P) \), we let \( \|f\|_2 = \sqrt{\int f^2 dP} \) denote its \( L^2(P) \) norm and let \( \|f\|_N = \sqrt{\frac{1}{N} \sum_{i=1}^M \sum_{j=1}^{n_i} f^2(x_{ij})} \) denote its empirical \( L^2(P_N) \) norm. Throughout this paper, we use \( c, c_1, \ldots \) to denote absolute constants. For ease of exposition, the specific values of these absolute constants might vary across different concrete contexts in this paper.

3 Recursive Dynamics of FedAvg and FedProx

Note that we can write \( f_t(x) = \langle \phi(x), \theta_t \rangle \), where \( \theta_t \) is the global model at the end of round \( t \). Let \( \theta_{i,t} \) denote the local updated model reported by worker \( i \) at round \( t \). By the aggregation rule at the parameter server, we know that

\[
\theta_t = \sum_{i=1}^M w_i \theta_{i,t},
\]

where the weight \( w_i = \frac{n_i}{N} \). Let \( \tilde{f}_t \in \mathbb{R}^N \) denote the resulting prediction value on the observed data:

\[
\tilde{f}_t = \begin{bmatrix} f_t(X_1) \\ \vdots \\ f_t(X_M) \end{bmatrix},
\]

where \( f_t(X_i) \in \mathbb{R}^{n_i} \) is a column vector whose \( j \)-th element is given by \( f_t(x_{ij}) \).

In this section, we derive compact matrix form expressions for the recursive dynamics of \( \theta_t \) and \( \tilde{f}_t \) under FedAvg and FedProx, respectively. As we will see, such matrix form expressions enable us to prove the convergence to the optimal error rate in the next section. As mentioned in Section 1, our expressions are by no means easy to obtain. Previous studies [ZWSL10, Sti18, KKM+20, LSZ+18] often imposed strong assumptions that are hard to justify and, more importantly, the simplified dynamics under those assumptions fail to capture the intricate interplay between the local gradient updates and the global averaging step.

3.1 Recursive dynamics of \( \theta_t \)

The following quantities will be used. Let \( \eta_i = \eta/n_i \). Define

\[
\gamma = \eta \max_{1 \leq i \leq M} \frac{\|\phi(X_i)\|_2^2}{n_i}
\]

and

\[
\kappa = \begin{cases} 
\frac{-\gamma_s}{1 - (1 - \gamma)^s} & \text{for FedAvg} \\
1 + \gamma & \text{for FedProx}
\end{cases}
\]

Intuitively, \( \kappa \) captures the stability of the local gradient update. For FedAvg, we need to choose the step size \( \eta \) so that \( \gamma \leq 1 \) and hence the local gradient update does not blow up. It is worth
noting that $\kappa \geq 1$ as long as $\gamma \leq 1$. Furthermore, when the step size $\eta$ is chosen so that $\gamma s$ is a small constant, $\kappa$ is close to 1.

The following two matrices arise naturally in the dynamics of model parameters $\theta_t$, as evident in Proposition 1. Define $A : \ell^2(N) \to \ell^2(N)$ to be the linear operator such that

$$A = \begin{cases} \sum_{i=1}^{M} w_i (I - \eta i \phi(X_i) \phi(X_i))^s & \text{for FedAvg,} \\ \sum_{i=1}^{M} w_i [I + \eta i \phi(X_i) \phi(X_i)]^{-1} & \text{for FedProx.} \end{cases}$$

Define $B : \mathbb{R}^N \to \ell^2(N)$ to be the linear operator such that $B = [B_1, \ldots, B_M]$, where

$$B_i = \begin{cases} \sum_{k=0}^{s-1} w_i [I - \eta i \phi(X_i) \phi(X_i)]^k \eta i \phi(X_i) \phi(X_i)^\top & \text{for FedAvg,} \\ w_i [I + \eta i \phi(X_i) \phi(X_i)]^{-1} \eta i \phi(X_i) \phi(X_i)^\top & \text{for FedProx.} \end{cases}$$

**Proposition 1.** For both FedAvg and FedProx, $\theta_t$ satisfies the following recursion:

$$\theta_t = A \theta_{t-1} + B y.$$  \hspace{1cm} (8)

Furthermore, for any given $\theta^* \in \ell^2(N)$, define

$$\Delta_{\theta^*} = \begin{bmatrix} \phi(X_1) (\theta^*_1 - \theta^*) \\ \vdots \\ \phi(X_M) (\theta^*_M - \theta^*) \end{bmatrix}.$$  \hspace{1cm} (9)

Then

$$\theta_t - \theta^* = A (\theta_{t-1} - \theta^*) + B \xi + B \Delta_{\theta^*}.$$  \hspace{1cm} (10)

**Remark 1.** Note that $\Delta_{\theta^*}$ captures the effect of the model heterogeneity. As we will see in Section E.3 when $\phi(x)$ is finite-dimensional, there always exists a unique choice of $\theta^*$ (cf. (25)) under which $B \Delta_{\theta^*} = 0$ and hence $\theta_t$ converges to $\theta^*$.

The expressions of matrices $A$ and $B$ are quite involved and analyzing the iterates in (8) or (10) is very challenging. Fortunately, after a careful examination of the structures of $A$, $B$, and the dynamics, we derive a collection of novel matrix inequalities in Section 3.3 which could be of independent interest in analyzing the first-order iterates. Those matrix identities enable us to write out alternative iterates that are much more tractable.

### 3.2 Recursive dynamics of $\vec{f}_t$

The dynamics of $\vec{f}_t$ are characterized in terms of the eigenvalues of the kernel matrix and a corresponding block diagonal matrix, formally defined next:

$$K = \frac{1}{N} \phi(X) \phi^\top(X) \in \mathbb{R}^{N \times N}.$$  \hspace{1cm} (11)

Let $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_N$ denote the eigenvalues of $K$ in descending order. Define $P \in \mathbb{R}^{N \times N}$ as a block diagonal matrix with the $i$-th diagonal block of size $n_i \times n_i$ given by

$$P_{ii} = \begin{cases} \sum_{k=0}^{s-1} [I - \eta i \phi(X_i) \phi(X_i)]^k & \text{for FedAvg,} \\ [I + \eta i \phi(X_i) \phi(X_i)]^{-1} & \text{for FedProx.} \end{cases}$$  \hspace{1cm} (12)

Note that FedAvg with $s = 1$ reduces to the usual gradient descent, where $P = I$ whose condition number is 1. In general, it can be shown (see (13)) that $\frac{\|P\|_2}{\lambda_{\min}(P)}$ — the condition number of $P$ — is upper bounded by $\kappa$ as defined in (5).
Proposition 2. For both FedAvg and FedProx, the prediction value satisfies the following recursion:

\[ \tilde{f}_t = [I - \eta KP] \tilde{f}_{t-1} + \eta KP y. \]  

Furthermore, for any given \( f^* \in \mathcal{H} \), define

\[ \Delta f^* = \begin{bmatrix} f_1^*(X_1) - f^*(X_1) \\ \vdots \\ f_M^*(X_M) - f^*(X_M) \end{bmatrix}. \]  

Then

\[ \tilde{f}_t - f^* = [I - \eta KP] (\tilde{f}_{t-1} - f^*) + \eta KP \xi + \eta KP \Delta f^*, \]  

where \( \tilde{f}^* \triangleq [f^*(X_1)^\top, \ldots, f^*(X_M)^\top]^\top \).

Remark 2. Note that \( \Delta f^* \) captures the effect of model heterogeneity to the dynamics of \( \tilde{f}_t \). Since for any \( f^* \in \mathcal{H} \), we can always write \( f^*(x) = \langle \phi(x), \theta^* \rangle \), it follows that \( \Delta f^* = \Delta \theta^* \).

3.3 Block Matrix Identities

We derive a set of block matrix identities which are crucial for us to derive the recursive dynamics of FedAvg and FedProx in Proposition 2. Those identities could be of independent interest to a broader audience.

Lemma 1. The following identities are true:

\[ B = \frac{\eta}{N} \phi^\top(X) P, \quad \phi(X) B = \eta K P, \quad B \phi(X) = I - A, \]  

and

\[ \phi(X) A = (I - \eta K P) \phi(X). \]  

4 Main Convergence Results

In this section we present our main results on the convergence of FedAvg and FedProx; the missing proofs can be found in the Appendices. Our results for FedAvg and FedProx can be compactly stated in a unified form where \( s \) is used. Recall that \( s \) is the algorithm parameter of FedAvg only. To recover the formal statements for FedProx, we need to set \( s = 1 \). For ease of exposition, without loss of generality, we assume \( f_0 = 0 \). Our results can be easily generalized to general \( f_0 \in \mathcal{H} \).

4.1 Convergence of prediction error in \( L^2(\mathbb{P}_N) \) norm

We first show that for both FedAvg and FedProx, the prediction error converges in \( L^2(\mathbb{P}_N) \) norm. Define the local empirical Rademacher complexity \([BBM05]\) as

\[ R_K(\epsilon) = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \min \{ \lambda_i, \epsilon^2 \}}. \]  

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Intuitively, $R_K(\epsilon)$ is a data-dependent complexity measure of the underlying RKHS and decreases with faster eigenvalue decay and smoother kernels. Define the critical radius as

$$\epsilon_N = \inf \left\{ \epsilon > 0 : R_K(\epsilon) \leq \frac{\epsilon^2}{\sqrt{2e\sigma}} \right\}. \quad (19)$$

The existence and uniqueness of $\epsilon_N$ is guaranteed for any RKHS [RWY14, Appendix D]. To avoid the possibility of over-fitting, we further choose the early stopping rule that

$$T = \left\lfloor \frac{1}{\epsilon_N^2 \eta s} \right\rfloor. \quad (20)$$

**Theorem 1.** For any $f^* \in \mathcal{H}$ such that $\|f^*\|_\mathcal{H} \leq 1$, it holds that

$$\mathbb{E}_\xi \left[ \|f_t - f^*\|_N^2 \right] \leq \frac{3\kappa}{\epsilon_N \eta s} + \frac{3\sqrt{\kappa}}{N} \|\Delta f^*\|_2^2, \quad \forall 1 \leq t \leq T.$$

Furthermore, if the coordinates of the noise vector $\xi$ are $N$ independent zero-mean and sub-Gaussian variables (with sub-Gaussian norm $\sigma$), then

$$\|f_T - f^*\|_N^2 \leq \frac{12\kappa \epsilon_N^2}{e} + \frac{3\kappa}{N} \|\Delta f^*\|_2^2 \quad (21)$$

with probability at least $1 - \exp\left(-cN\epsilon_N^2\right)$, where $c$ is a universal constant.

Theorem 1 implies that the prediction error decays as $1/t$ up to the stopping time $T$. Specializing our result to $s = 1$ recovers the existing convergence result of the centralized gradient descent with early stopping for non-parametric regression in [RWY14]. We remark that the convergence rate is expected to be $1/t$ instead of an exponential convergence in general, as the minimum eigenvalue $\lambda_N$ of the kernel matrix is not bounded away from 0 and may converge to 0 as $N$ diverges. In the special case where $\phi(X)$ is $d$-dimensional, the rank of $K$ is at most $d$ and hence $R_K(\epsilon) \leq \sqrt{d/N\epsilon}$. It follows that $\epsilon_N = \Theta(\sigma \sqrt{d/N})$. Moreover, when $N \geq d$, we expect $\lambda_d$ is bounded away from 0 and hence the prediction error converges exponentially. This special case is investigated in Section 4.3 where we show an even stronger convergence of the model parameter.

**Remark 3.** (Effect of local steps) Theorem 1 reveals an interesting trade-off between the accuracy and convergence speed in terms of the number of local steps $s$ for FedAvg. On one hand, when $s$ increases, the early stopping time $T$ shrinks and the convergence rate increases by a factor of $s$. This reduces the communication rounds in FedAvg by a factor of $s$. On the other hand, the prediction error increases by a factor of $\kappa$, which is an increasing function of $s$. Notably, when $s$ is relatively small so that $\gamma s$ is a small constant, $\kappa$ will be close to 1, in which case we can recoup the loss of the accuracy while enjoying the saving of the communication cost.

**Remark 4** (Intuition behind the early stopping rule). As evident from the proof of Theorem 1, the early stopping rule (20) is chosen to balance the bias and the variance. In particular, $T$ is chosen to the largest time index $t$ so that roughly the variance upper bound $\sigma^2\eta tsR_K^2(1/\sqrt{\eta ts})$ matches with the bias upper bound $\frac{1}{\eta ts}$. Also, from Lemma 3, we can clearly see that an early stopping is necessary for avoid over-fitting. If $t$ were tending infinity, the variance term would eventually rise up to $(1/N)\mathbb{E} \left[ \|\xi\|_2^2 \right] = \sigma^2$, fitting the noise entirely.
4.2 Convergence of prediction error in $L^2(\mathbb{P})$ norm

Next, we establish the convergence of prediction error in $L^2(\mathbb{P})$ norm when the design matrix $X$ is random. The convergence is characterized in terms of the eigenvalues of the kernel function $k(x, y)$. Let $\bar{\lambda}_1 \geq \bar{\lambda}_2 \geq \ldots \geq 0$ denote the eigenvalues of $k(x, y)$ in $L^2(\mathbb{P})$. Define the population analog of the local Rademacher complexity

$$\bar{R}_k(\epsilon) = \sqrt{\frac{1}{N} \sum_{i=1}^{\infty} \min\{\bar{\lambda}_i, \epsilon^2\}}.$$

and the population analog of the critical radius

$$\bar{\epsilon}_N = \inf\left\{ \epsilon > 0 : \bar{R}_k(\epsilon) \leq \frac{\epsilon^2}{2c\sigma} \right\}.$$

**Theorem 2.** Suppose that rows of $X$ are sampled i.i.d. according to distribution $\mathbb{P}$. The coordinates of the noise vector $\xi$ are $N$ independent zero-mean and sub-Gaussian variables (with sub-Gaussian norm $\sigma$). There exist universal constants $c_1, c_2, c_3$ such that with probability at least $1 - c_1 \exp\left(-c_2 N\bar{\epsilon}_N^2\right)$,

$$\|f_T - f^*\|^2_2 \leq c_3 \kappa \left(\frac{\bar{\epsilon}_N^2}{N} + \|\Delta \theta^*\|^2_2 / N\right).$$

It follows that $E_{X, \xi} \left[\|f_T - f^*\|^2_2\right] \leq c_4 \kappa \left(\bar{\epsilon}_N^2 + \|\Delta \theta^*\|^2_2 / N\right)$ for a constant $c_4$.

Notably, the noises $\xi$ are not necessarily identically distributed. An interesting intermediate step in establishing Theorem 2 is to show that $\|f_t\|_{H}$ (equivalently, $\|\theta_t\|_2$) is bounded with high probability; see Lemma 5 Appendix E for formal statements and a proof.

As immediate corollaries of Theorem 2, we show that both FedAvg (with $s \geq 1$) and FedProx achieve the centralized minimax-optimal estimation error rate for the following specific kernels [YB99, RJWY12].

**Finite rank kernels** Consider the class of RKHS with finite-rank kernels, that is, there exists a finite $r$ such that $\bar{\lambda}_j = 0$ for $j > r + 1$. For example, the kernel $k(x, y) = (1 + \langle x, y \rangle)^a$ for $x, y \in \mathbb{R}^d$ generates the RKHS of all multivariate polynomials of $2d$ variables and degree at most $2a$.

**Corollary 1.** Suppose in addition to the conditions of Theorem 2 the kernel $k$ has finite rank $r$. Then

$$E_{X, \xi} \left[\|f_T - f^*\|^2_2\right] \leq c_3 \kappa \sigma^2 \frac{r}{N}$$

for some universal constant $c_3 > 0$.

**Kernels with polynomial eigenvalue decay** Consider the kernels whose eigenvalues exhibit a polynomial decay with exponent $\beta$, that is,

$$\bar{\lambda}_i \leq Ci^{-2\beta} \quad \text{for } \beta > 1/2 \text{ and a constant } C > 0. \quad (22)$$

For example, the first-order Sobolev kernel $k(x, y) = \min\{x, y\}$ on the unit square $[0, 1]^2$ satisfies the eigenvalue decay (22) with $\beta = 1$.

**Corollary 2.** Suppose in addition to the conditions of Theorem 2 the kernel $k$ satisfies (22). Then

$$E_{X, \xi} \left[\|f_T - f^*\|^2_2\right] \leq c_3 \kappa \left(\frac{\sigma^2}{N}\right)^{2\beta/(2\beta+1)} \quad (23)$$

for some universal constant $c_3 > 0$. 

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4.3 Convergence of model parameter in $\ell^2$ norm

Note that $f_t(x) = \langle \phi(x), \theta_t \rangle$ and hence $\|f_t\|_H = \|\theta_t\|_2$. In Section 4.2, we show the prediction error convergence in $L^2(\mathbb{P})$ norm and the statistical optimality of our characterization for a couple of popular kernel families. In this section, we relax the i.i.d. assumption on the random design matrix $X$ and show convergence in $\ell^2$ norm – a much stronger mode of convergence. We assume that $\phi(x)$ is finite-dimensional and $\phi(X)^\top \phi(X)$ is positive definite. This encompasses the popular random feature model which maps the input data to a randomized low-dimensional feature space [RR+07].

**Theorem 3.** Suppose that $\phi(x)$ is $d$-dimensional and that $\rho = \lambda_{\min}(\phi(X)^\top \phi(X))/N > 0$. Then
\[
E_\xi \left[ \|\theta_t - \theta^*\|_2^2 \right] \leq \left( 1 - \frac{s\eta \rho}{\kappa} \right)^{2t} \|\theta^*\|_2^2 + \sigma^2 \frac{\kappa d}{N \rho},
\]  
(24)

where
\[
\theta^* = (I - A)^{-1} B \begin{bmatrix} \phi(X_1)\theta_1^* \\ \vdots \\ \phi(X_M)\theta_M^* \end{bmatrix}.
\]  
(25)

Moreover,
\[
\|\theta^* - \theta_j^\ast\|_2 \leq \Delta \sqrt{\frac{\kappa}{N \rho} \sum_{i=1}^M \|\phi(X_i)\|_2^2} \quad \forall 1 \leq j \leq M,
\]  
(26)

where $\Delta = \max_{i,j} \left\| f_i^\ast - f_j^\ast \right\|_{\mathcal{H}} = \max_{i,j} \left\| \theta_i^\ast - \theta_j^\ast \right\|_2$.

Note that, in general, the assumption $\rho > 0$ is necessary for the underlying model parameters to be uniquely identifiable. The conclusions (24) and (26) together imply that both FedAvg and FedProx converge exponentially fast to some $\theta^*$ that is close to the local model parameter $\theta_j^\ast$ as long as the model heterogeneity $\Delta$ is moderate. When the feature matrix $\phi(X)$ is random with independent rows, we have the following more explicit result.

**Corollary 3.** Suppose that $\phi(X)$ are $N \times d$ matrix whose rows are independent sub-Gaussian isotropic random vectors in $\mathbb{R}^d$. There exist universal constants $c_1, c_2$ such that if $N \geq c_1 d$, then with probability at least $1 - e^{-d}$,
\[
E_\xi \left[ \|\theta_t - \theta^*\|_2^2 \right] \leq \left( 1 - \frac{s\eta \sqrt{2}\kappa}{\sqrt{d}} \right)^{2t} \|\theta^*\|_2^2 + \sigma^2 \frac{\kappa d}{N}
\]  
(27)

and
\[
\|\theta^* - \theta_j^\ast\|_2 \leq c_1 \kappa \Delta \left( 1 + \sqrt{\frac{Md}{N}} \right).
\]  
(28)

Corollary 3 accommodates data heterogeneity, where the rows of $X$ can be non-identically distributed as long as the covariance matrix is the identity matrix. One can further relax the assumption to allow for distinct covariance matrices, which we will discuss in the next paragraph. Note that the rate $d/N$ in (27) is minimax-optimal for estimating an $d$-dimensional vector in the centralized setting. Furthermore, the impact of the model heterogeneity $\Delta$ is quantified in (28). As long as the average sample size per worker $N/M$ is comparable to the dimension $d$, $\|\theta^* - \theta_j^\ast\|_2$ is on the order of $\Delta$. Somewhat surprisingly, this implies that even when the local sample size $n_j$ is much smaller than dimension $d$, worker $j$ can still accurately estimate $\theta_j^\ast$, to some extent, by participating in FL. We study the benefits of joining FL formally in the next subsection.
**Distinct covariance matrices: Subspace model** One interesting instance of distinct covariance matrices is subspace models, wherein rows of $\phi(X)$ are drawn from possibly different subspaces of low dimensions. This instance captures a wide range of popular FL applications such as image classification wherein different workers collect different collections of images \cite{MMR17}. Concretely, in image classification, some workers may only have images related to airplanes or automobiles, while others have images related to cats or dogs. It is of great interest to “pool” the local data and train a global model that can distinguish all the different classes. Formally, we consider the following subspace model.

**Definition 1** (Subspace model). Suppose that the rows of $\phi(X_i)$ lie in a subspace of dimension $r_i$, that is,

$$\phi^\top(X_i) = U_i F_i^\top$$

where $U_i \in \mathbb{R}^{d \times r_i}$ such that $U_i^\top U_i = I$, and $F_i \in \mathbb{R}^{n_i \times r_i}$.

**Corollary 4.** Suppose that $\phi(X)$ follows the subspace model in Definition 1, where $U_i$’s are independent and $\mathbb{E} \left[U_i U_i^\top \right] = \frac{d}{N} I_d$. Moreover, assume that

$$\lambda_{\min}(F_i^\top F_i) \geq \alpha \frac{n_i d}{r_i}, \quad \forall 1 \leq i \leq M,$$

for some $\alpha > 0$. Let $\nu = \max_{i \in [M]} n_i / r_i$. Choose the step size $\eta < \min_{i \in [M]} \frac{n_i}{F_i^\top F_i}$. There exists a constant $C$ such that if $N \geq C d \log d$, then with probability at least $1 - 1/d$,

$$\mathbb{E} \left[\|\theta_t - \theta^*\|_2^2\right] \leq \left(1 - \frac{s \eta \alpha}{2\nu}\right)^{2t} \|\theta^*\|_2^2 + \sigma^2 \frac{2\kappa d}{N\alpha}$$

Moreover, if

$$\|F_i^\top F_i\|_2 \leq \beta \frac{n_i d}{r_i}, \quad \forall 1 \leq i \leq M,$$

then with probability at least $1 - 1/d$,

$$\|\theta_t - \theta^*\|_2 \leq \Delta \sqrt{\frac{2\kappa \beta \nu \alpha d}{\alpha N}}.$$

**Remark 5.** Note that (30) is imposed to ensure that the local data at worker $i$ contains strong enough signal about $\theta^*_i$ on every dimension of the subspace given by $U_i$. To appreciate the intuition behind (30), it is instructive to consider the following two examples:

- **Orthogonal local dataset:** Suppose that the rows of $\phi(X_i)$ are orthogonal to each other and each of which has Euclidean norm $\sqrt{d}$. In this case, we have $r_i = n_i$ and $F_i = \sqrt{d} I_{r_i}$. Therefore, $\alpha = 1$ and $\nu = 1$. Then Corollary 4 implies that as long as $N \geq C d \log d$, $\theta^t$ converges exponentially fast to $\theta^*$ up to the optimal mean-squared error rate $d/N$.

- **Gaussian local dataset:** Suppose that the rows of $\phi(X_i)$ are i.i.d. $\mathcal{N}(0, U_i \Sigma U_i^\top)$. In other words, $\phi^\top(X_i) = U_i F_i^\top$, where the rows of $F_i$ are i.i.d. $\mathcal{N}(0, \Sigma_i^1/2)$. Consider the simple special case where $\Sigma_i = \frac{d}{r_i} I_{r_i}$, so that $\text{Tr}(\Sigma_i) = d$ and hence each row of $\phi(X_i)$ has the squared Euclidean norm $d$ on average. In this case, by Gaussian concentration inequality \cite[Theorem 5.39]{Ver10}, with high probability $1 - \delta \leq \alpha \leq \beta \leq 1 + \delta$ for some small constant $\delta > 0$, provided that $n_i \geq C \max\{r_i, \log M\}$ for some sufficiently large constant $C$. Then Corollary 4 implies that if further $N \geq C d \log d$, $\theta_t$ converges exponentially fast to $\theta^*$ up to the optimal mean-squared error rate $d/N$. Note that here we pay an extra factor of $\nu$ in the sample complexity. This is necessary in general. To see this, consider the extreme case where $r_i = 1$ and $n_i = n$, i.e., all local data at worker $i$ lie on a straight line in $\mathbb{R}^d$. Then by the standard coupon collector’s problem, we need $M \geq d \log d$ in order to sample all the $d$ basis vectors in $\mathbb{R}^d$. ...
4.4 Characterization of federation gains

In this section, we characterize the federation gains in the presence of covariate and response heterogeneity. Formally, given an estimator \( \hat{\theta}_j \) based on the local data \((X_j, y_j)\) at worker \( j \), define its (worst-case) risk and minimax risk as

\[
R_j (\hat{\theta}_j) = \sup_{\theta_j^* \in \Theta} \mathbb{E}_{X_j, \xi_j} \left[ \|\hat{\theta}_j - \theta_j^*\|_2^2 \right], \quad R^*_j = \inf_{\hat{\theta}_j} R (\hat{\theta}_j),
\]

respectively, where \( \Theta \) denotes the unit ball in \( \mathbb{R}^d \).

**Definition 2** (Federation gain). The federation gain of worker \( i \) in participating FL is defined as the ratio of the local minimax risk \( R_j \) and the limiting risk achievable by \( \theta_t \):

\[
FG_j = \lim_{t \to \infty} \frac{R^*_j}{R_j (\theta_t)}.
\]

Recall that \( \theta_t \) is the model trained under FL after \( t \) rounds. Intuitively, the federation gain is the multiplicative reduction of the mean-squared error of estimating \( \theta_j^* \) in joining FL compared to the best local estimators.

It can be shown that (see e.g. [Mou19])

\[
R^*_j \geq \begin{cases} 
(1 - n_j/d) \|\theta_j^*\|_2^2 & \text{if } n_j < d \\
\sigma^2 d/n_j & \text{if } n_j \geq d.
\end{cases}
\]

Combining the above with Corollary [3] we immediately have the following theorem.

**Theorem 4.** Consider the same setup as Corollary [3]. Then for \( 1 \leq j \leq M \), there exists a universal constant \( c_1 > 0 \) such that

\[
FG_j \geq \begin{cases} 
c_1 \frac{\sigma^2 d/n_j}{(1-n_j/d) \|\theta_j^*\|_2^2} & \text{if } n_j \geq d \\
c_1 \sigma^2 d/n_j + \Delta^2 (1+Md/N) & \text{if } n_j < d.
\end{cases}
\]

(33)

**Remark 6.** Theorem 4 reveals interesting observations on the federation gain. On the extreme case where \( \Delta = 0 \), i.e., all the local model parameters \( \theta_i^* \) are the same, the federation gain achieves its maximum, which is at least on the order of \( \min\{N/n_j, N/d\} \). As the model heterogeneity \( \Delta \) increases the federation gain decreases. In particular, suppose the average number of local data \( N/M \gtrsim d \). For data-scarce workers with local data volume \( n_j < d \), the federation gain is at least on the order of \( \sigma^2 d/n_j \), which exceeds one when \( \Delta \leq \sigma \sqrt{d/n_j} \). For data-rich workers with local data volume \( n_j \geq d \), the federation gain is at least on the order of \( \sigma^2 d/(n_j \Delta^2) \), which exceeds one when \( \Delta \leq \sigma \sqrt{d/n_j} \).

**Remark 7** (Federation gain under subspace model). Corollary 4 allows us to quantify the federation gain in the presence of covariate heterogeneity. Specifically, suppose that \( \alpha \) is a fixed positive constant and \( \theta_i^* = \theta^* \) for all \( i \in [M] \). Then (31) implies that when \( N \geq C \nu d \log d \), \( \theta_t \) converges exponentially fast to the mean-squared error rate \( \sigma^2 d/N \). On the contrary, since the local data at worker \( j \) lie in an \( r_j \)-dim space uniformly chosen at random. Thus, the minimax-optimal mean-squared error (MSE)
is at least on the order of $(1-r_j/d)\|\theta^*\|^2_2 + \sigma^2 d/n_j$. Therefore, the federation again at worker $j$ satisfies

$$\text{FG}_j \geq c_1 \frac{(1-r_j/d)\|\theta^*\|^2_2 + \sigma^2 d/n_j}{\sigma^2 d/N}, \quad \text{if } N \geq C\nu d \log d.$$ 

for some constant $c_1$. More specifically,

- For data-scarce workers with local data volume $n_j \ll d$, $\text{FG}_j$ is dominated by $N/n_j$, which is unchanged with $r_j$.
- For data-rich workers with local data volume $n_j \gg d$, $\text{FG}_j$ is dominated by $\frac{(1-r_j/d)\|\theta^*\|^2_2}{\sigma^2 d/N}$, which is decreasing in $r_j$.

If instead $N \ll \nu d \log d$, we expect that $\theta_t$ do not estimate $\theta^*$ well and hence the Federation gain will be small. In conclusion, the Federation gain will exhibit a sharp jump at a critical sample complexity $N = \Theta(\nu d \log d)$. This is confirmed by our numerical experiment in Section 5.3.

5 Experimental Results

In this section, we provide experimental results corroborating our theoretical findings.

5.1 Stationary points and estimation errors

We numerically verify that despite the failure of converging to the stationary points of the global empirical risk function, both FedAvg and FedProx can achieve low estimation errors.

We adopt the same simulation setup of [PW20] for fairness in comparison. The impacts of using minibatch on the achievability of stationary points and on the estimation errors of FedAvg and FedProx can be found in Appendix B. We let $M = 25$, $d = 100$, and $n_i = 500$. For each worker $i$, $f_i^* = X_i\theta^*$ for some $\theta^* \in \mathbb{R}^d$ and the response vector $y_i = (y_{ij}) \in \mathbb{R}^{n_i}$ is given by $y_i = X_i\theta^* + \xi_i$, where $\xi_i = (\xi_{ij}) \in \mathbb{R}^{n_i}$ follows $\mathcal{N}(0, \sigma^2 I)$ with $\sigma = 0.5$. The local design matrices $X_i$ are independent random matrices with i.i.d. Gaussian $\mathcal{N}(0, 1)$ entries. Let $L(\theta) = \sum_{i=1}^M \|y_i - X_i\theta\|^2_2$ denote the global empirical risk function. The difference to [PW20] is that, instead of plotting the sub-optimality in the excess risk $L(\theta_t) - \min_{\theta} L(\theta)$, we plot the trajectories of $\|\nabla L(\theta_t)\|_2$ to highlight the unreachability to stationary points of $L(\theta_t)$.

For both FedAvg and FedProx, we choose the step size $\eta = 0.1$. Fig. 1A confirms the observation in [PW20] that FedAvg with $(s \geq 2)$ and FedProx fail to converge to the stationary point of global empirical risk function $L(\theta)$. Surprisingly, Fig. 1B shows that $\|\theta_t - \theta^*\|_2$ converges to the optimal estimation error rate. In particular, both FedAvg with $s = 5, 10$ and FedProx can achieve the same low error as FedAvg with $s = 1$, i.e., the standard centralized gradient descent method.

5.2 Federation gains versus model heterogeneity

Complementing our Theorem 4, we provide a numerical study on the federation gain.

We build on our previous experiment setup by allowing for unbalanced local data and the heterogeneity in $f_i^*$. We choose $M = 20$, $d = 100$, $n_i = 50$ for half of the workers, and $n_i = 500$ for the remaining workers. We refer to the workers with $n_i = 50$ as data scarce workers, and to the others as data rich workers. We run the experiments with a prescribed set of heterogeneity levels. All the other specifications are the same as before.

We randomly choose a data scarce worker and a data rich worker, and plot the federation gains against the model heterogeneity $\Delta = \max_{i,j \in [M]} \|\theta^*_i - \theta^*_j\|_2$ in Fig. 2. Note that in evaluating the
federation gains, we use the minimum-norm least squares as the benchmark local estimator, that is \( \hat{\theta}_j = (X_j^T X_j)^+ X_j^T y_j \), where the symbol + denotes the Moore-Penrose pseudoinverse. It is known that this estimator can attain the minimax-optimal estimation error rate \([Mon19]\). We see that consistent

\[
\begin{align*}
\text{gain} & = 1 - \frac{n_j}{d} \left\| \frac{\theta_j}{\theta^*} \right\|_2 \\
\Delta & = \frac{d}{n_j}
\end{align*}
\]

Figure 2: Federation gains versus \( \Delta \). A data scarce worker benefits more from FL participation.

with our theory, despite the difference in the training behaviors, the models trained under \text{FedAvg} with different choices of aggregation periods \( s \) and under \text{FedProx} have almost indistinguishable federation gains. Moreover, as predicted by our theory, the federation gain drops with increasing model heterogeneity \( \Delta \), while the federation gain of the data scarce worker is much higher than that of the data rich worker. Recall that the federation gain exceeds 1 if and only if the FL model is better than the locally trained model. We observe that the federation gain of a data scarce worker drops below 1 at \( \Delta \approx 7.5 \), whereas the federation gain of a data rich worker drops below 1 at \( \Delta \approx 0.3 \). These numbers turn out to be closely match with our theoretically predicted thresholds given in Remark 6, which are \( \Delta \approx \sqrt{1 - n_j/d} \left\| \frac{\theta_j}{\theta^*} \right\|_2 \approx 7 \) and \( \Delta \approx \sigma \sqrt{d/n_j} \approx 0.22 \), respectively.

5.3 Federation gain versus covariate heterogeneity

As mentioned in Section 2, data heterogeneity includes both response heterogeneity (a.k.a. concept shift) and covariate heterogeneity (a.k.a. covariate shift). Our theory in Section 4.4 applies to both types of data heterogeneity. Due to space limitations, Section 5.2 illustrates the tradeoff between federation gain and response heterogeneity only and Theorem 4 is stated for the family of distributions with isotropic covariance matrix. As commented in the paragraph following Corollary 3, our results can be generalized to distinct covariance matrices. Hence, in this subsection we present our experimental results on the subspace models which capture interesting FL applications such as images classification wherein different workers keep different subcollections of images \([MMR+17]\). The formal definition of the subspace model and relevant results can be found in Definition 4, Corollary 4, Remark 5, and Remark 7.

In our experiments, we choose \( M = 20 \), \( d = 100 \), \( \sigma = 0.5 \), \( n_i = 50 \) for half of the workers, and \( n_i = 500 \) for the remaining workers. We let the 20 workers share a common underlying truth, i.e., \( \theta_j^* = \theta^* \) for all \( j \), which is randomly drawn from \( \mathcal{N}(0, I) \). The responses \( y_i \) are given as \( y_i = X_i \theta^* + \xi_i \). The design matrices \( X_i \in \mathbb{R}^{n_i \times d} \) at the workers lie in different subspaces of dimension \( k \); here \( k \) ranges from 1 to 100. Specifically, \( X_i \)'s are generated as follows: we first generate a random index set \( E \subseteq \{1, \ldots, d\} \) of cardinality \( k \), and generate a matrix \( X_i \) with each row independently distributed as
$N(0, \frac{d}{k}I_E)$, where $I_E$ is a diagonal matrix with $(I_E)_{ii} = 1_{\{i \in E\}}$. The scaling $\frac{d}{k}$ ensures that each row of $X_i$ has $\ell^2$ norm $\sqrt{d}$ in expectation and hence the signal-to-noise ratio is consistent across different values of $k$. As $\|X_i\|_2$ increases by a factor of $\sqrt{d/k}$, we rescale the stepsize by choosing $\eta = 0.1/\left(\frac{d}{k}\right)$ for the stability of local iterations, according to Corollary 4. Notably, when $k = d$, the stepsize becomes $\eta = 0.1$ which is the same as Section 5. We randomly choose a data scarce worker and a data rich worker and record the federation gains. We plot the average federation gains over 20 trials against $k$ – dimension of the subspaces – in Fig. 3. We have the following key observations:

- First, for any fixed $k$, a worker’s federation gains of the model trained by FedAvg with $s = 1, 5, 10$ and FedProx are almost identical. This is consistent with our theory, as we show both FedAvg and FedProx converge to the minimax-optimal mean-squared error rate $d/N$ in Corollary 4.

- Second, up to $k \approx 27$, the curves for the data scarce and the data rich workers are roughly the same. This is because when $k \leq 27$, the main “obstacle” in learning $\theta^*$ is the lack of sufficient coverage of each of the 100 dimensions by the data collectively kept by the 20 workers.

- Third, for both curves there are significant jumps starting when $k \approx 16$ to when $k \approx 23$. If we can pool the data together, due to the coupon-collecting effect, as soon as $M \times k \geq d \log d \approx 460$, all the $d$ dimensions can be covered by the design matrices and hence the underlying truth $\theta^*$ can be learned with high accuracy. Since $M = 20$, this explains the significant jumps in federations gains in Fig. 3 when $k$ is around 23.

- Finally, the curve trends are different for data scarce and data rich workers. For a data scarce worker, as shown in Fig. 3a, as $k$ increases, the federation gain first increases and then stabilizes around 107. In contrast, for a data rich worker, as shown in Fig. 3b, as $k$ increases, the federation gain first increases and then quickly decreases when $k$ approaches 100. This distinction is because a data scarce worker, on its own, cannot learn $\theta^*$ well as $n_i = 50 \ll 100$ no matter how large $k$ is, while a data rich has 500 data tuples and can learn $\theta^*$ on its own quite well when $k$ approaches 100.

These empirical observations are consistent with our theoretical predictions in Remark 5 and Remark 7.
5.4 Fitting nonlinear functions

In this section, we go beyond linear models and consider fitting nonlinear models. In particular, we focus on fitting $U_5$ – the degree-5 Chebyshev polynomials of the second kind, which is a special case of the Gegenbauer polynomials and has the explicit expression

$$U_5(x) = 32x^5 - 32x^3 + 6x.$$ 

We choose the feature map $\phi(x) = [1, x, \ldots, x^5]^\top$ to be the monomial basis up to degree 5 and run FedAvg and FedProx on the polynomial coefficients. We consider $M = 20$ workers and equal size local dataset $n_i \in \{1, 2, \ldots, 10\}$. Correspondingly, the global dataset size ranges from 20 to 200 as indicated by Fig.4. The response value is given as $y = U_5(x) + \xi$ where $\xi \sim \mathcal{N}(0, \sigma^2)$ with $\sigma = 0.5$. We consider heterogeneous local datasets. Specifically, each worker $i \in [M]$ probes the function on disjoint intervals $[-1 + \frac{2i-1}{M}, -1 + \frac{2i}{M})$. In the experiments, we generate covariates $x_{ij}$ using the uniform grid. For the fitted function $\hat{f}$, we evaluate the mean-squared error (MSE) as

$$\| \hat{f} - f^* \|_2^2 = \int_{-1}^{1} |\hat{f}(x) - f^*(x)|^2 \, dx.$$ 

We run FedAvg and FedProx with the same stepsize $\eta = 0.1$ as before, and evaluate the MSE via Monte Carlo integration. We plot the average MSE over 500 trials.

![Graph](image)

(a) Estimation errors 
(b) Reciprocal of estimation errors

Figure 4: Estimation errors of fitting polynomials

As shown by Fig.4a, the four curves of the model prediction errors under FedAvg with different choices of $s$ and FedProx are very similar. To test our theoretical prediction on the statistical rates stated in Corollary 1, we plot the reciprocal of prediction errors in Fig.4b. Though the differences in the reciprocal of the prediction errors get amplified as the errors approach zero, each of the four curves in Fig.4b are mostly straight lines. Moreover, the four curves have similar slopes with the slope of $s = 10$ being slightly smaller than others. This is because a larger $s$ leads to a $\kappa$ being slightly greater than one and thus an increased error as predicted by Corollary 1.

References

[BBM05] Peter L Bartlett, Olivier Bousquet, and Shahar Mendelson. Local rademacher complexities. *The Annals of Statistics*, 33(4):1497–1537, 2005.
Fei Chen, Mi Luo, Zhenhua Dong, Zhenguo Li, and Xiuqiang He. Federated meta-learning with fast convergence and efficient communication. *arXiv preprint arXiv:1802.07876*, 2018.

Yuyang Deng, Mohammad Mahdi Kamani, and Mehrdad Mahdavi. Adaptive personalized federated learning. *arXiv preprint arXiv:2003.13461*, 2020.

Canh T Dinh, Nguyen H Tran, and Tuan Dung Nguyen. Personalized federated learning with moreau envelopes. *arXiv preprint arXiv:2006.08848*, 2020.

Alireza Fallah, Aryan Mokhtari, and Asuman Ozdaglar. Personalized federated learning: A meta-learning approach. *arXiv preprint arXiv:2002.07948*, 2020.

Roger A Horn and Charles R Johnson. *Matrix analysis*. Cambridge university press, 2012.

Yihan Jiang, Jakub Konečný, Keith Rush, and Sreeram Kannan. Improving federated learning personalization via model agnostic meta learning. *arXiv preprint arXiv:1909.12488*, 2019.

Sai Praneeth Karimireddy, Satyen Kale, Mehryar Mohri, Sashank Reddi, Sebastian Stich, and Ananda Theertha Suresh. Scaffold: Stochastic controlled averaging for federated learning. In *International Conference on Machine Learning*, pages 5132–5143. PMLR, 2020.

Peter Kairouz, H Brendan McMahan, Brendan Avent, Aurélien Bellet, Mehdi Bennis, Arjun Nitin Bhagoji, Keith Bonawitz, Zachary Charles, Graham Cormode, Rachel Cummings, et al. Advances and open problems in federated learning. *arXiv preprint arXiv:1912.04977*, 2019.

Jakub Konečný, H Brendan McMahan, Daniel Ramage, and Peter Richtárik. Federated optimization: Distributed machine learning for on-device intelligence. *arXiv preprint arXiv:1610.02527*, 2016.

Jakub Konečný, H Brendan McMahan, Felix X Yu, Peter Richtárik, Ananda Theertha Suresh, and Dave Bacon. Federated learning: Strategies for improving communication efficiency. *arXiv preprint arXiv:1610.05492*, 2016.

Tian Li, Anit Kumar Sahu, Manzil Zaheer, Maziar Sanjabi, Ameet Talwalkar, and Virginia Smith. Federated optimization in heterogeneous networks. *arXiv preprint arXiv:1812.06127*, 2018.

Sen Lin, Guang Yang, and Junshan Zhang. A collaborative learning framework via federated meta-learning. In *2020 IEEE 40th International Conference on Distributed Computing Systems (ICDCS)*, pages 289–299. IEEE, 2020.

Brendan McMahan, Eider Moore, Daniel Ramage, Seth Hampson, and Blaise Agueray Arcas. Communication-efficient learning of deep networks from decentralized data. In *Artificial Intelligence and Statistics*, pages 1273–1282. PMLR, 2017.

Jaouad Mourtada. Exact minimax risk for linear least squares, and the lower tail of sample covariance matrices. *arXiv preprint arXiv:1912.10754*, 2019.
[PW20] Reese Pathak and Martin J Wainwright. Fedsplit: An algorithmic framework for fast federated optimization. arXiv preprint arXiv:2005.05238, 2020.

[RJWY12] Garvesh Raskutti, Martin J Wainwright, and Bin Yu. Minimax-optimal rates for sparse additive models over kernel classes via convex programming. Journal of Machine Learning Research, 13(2), 2012.

[RR+07] Ali Rahimi, Benjamin Recht, et al. Random features for large-scale kernel machines. In NIPS, volume 3, page 5. Citeseer, 2007.

[RV+13] Mark Rudelson, Roman Vershynin, et al. Hanson-wright inequality and sub-gaussian concentration. Electronic Communications in Probability, 18, 2013.

[RWY14] Garvesh Raskutti, Martin J Wainwright, and Bin Yu. Early stopping and non-parametric regression: an optimal data-dependent stopping rule. The Journal of Machine Learning Research, 15(1):335–366, 2014.

[Sti18] Sebastian U Stich. Local sgd converges fast and communicates little. arXiv preprint arXiv:1805.09767, 2018.

[Ver10] R. Vershynin. Introduction to the non-asymptotic analysis of random matrices. Arxiv preprint arxiv:1011.3027, 2010.

[Wai19] Martin J Wainwright. High-dimensional statistics: A non-asymptotic viewpoint, volume 48. Cambridge University Press, 2019.

[YB99] Yuhong Yang and Andrew Barron. Information-theoretic determination of minimax rates of convergence. Annals of Statistics, pages 1564–1599, 1999.

[ZLL+18] Yue Zhao, Meng Li, Liangzhen Lai, Naveen Suda, Damon Civin, and Vikas Chandra. Federated learning with non-iid data. arXiv preprint arXiv:1806.00582, 2018.

[ZWSL10] Martin Zinkevich, Markus Weimer, Alexander J Smola, and Lihong Li. Parallelized stochastic gradient descent. In NIPS, volume 4, page 4. Citeseer, 2010.
Appendices

A Detailed Descriptions of FedAvg and FedProx

Recall that $f^*_i \in \mathcal{H}$ and hence there exists $\theta^*_i \in \ell^2(N)$ such that $f^*_i(x) = \langle \phi(x), \theta^*_i \rangle$. To implement the functional gradient descent and functional proximal updates, one common practice in large-scale distributed computing is to choose a feature map $\phi$ based on the given kernel $k$ and then focus on updating $\theta$. For example, for polynomial kernels the feature map is often selected as the monomial basis up to the given degree; for Gaussian kernels the feature map becomes the monomial basis weighted by the Gaussian density, and the approximation by the random Fourier features is a popular choice $[RR+07]$. Though the practical choice of $\phi$ is often of finite dimension, most of our results work for infinite dimension as well.

Detailed implementations of FedAvg $[MMR+17]$ and FedProx $[LSZ+18]$ involve multiple tuning parameters, such as worker sampling rate $C \in (0, 1]$ and minibatch size $B$. Specifically, $C$ represents the fraction of workers recruited in each communication round with $C = 1$ meaning each of the $M$ workers is recruited in the entire model training model, and $B$ is the number of data samples used in each local model update. In practice, when the total number of workers is huge, $C$ is often chosen to be strictly less than 1. In our experiments, due to resource limitation, we consider small $M$ and choose $C = 1$. We simulate the impacts of the minibatch size on the convergences of FedAvg and FedProx. Nevertheless, to provide a focus and for analysis tractability, our analysis is derived for the algorithm backbones presented in Section 2.1.

For clarity, for each of the algorithm (FedAvg or FedProx), we provide the programs at the parameter server and each of the chosen worker in a round separately. Recall that the local dataset on worker $i$ is denoted by $S_i$. We denote the local empirical risk over a minibatch $b \subseteq S_i$ is denoted by $L_i(\theta; b)$.

A.1 FedAvg $[MMR+17]$

In FedAvg, the program executed by the parameter server (i.e., FedServer $[1]$) has the following inputs: $\theta_0$ – model initialization; $C \in (0, 1]$ – client recruitment fraction; $N$ – the total number of data points available for training; $n_i$ for $i \in [M]$ – size of local datasets of each worker; $T$ – the termination round.

| FedLServer 1: FedAvg: Parameter server |
|---------------------------------------|
| **Input:** $\theta_0, C \in (0, 1], N, T, n_i$ for $i \in [M]$; |
| **Output:** $\theta_T$ |
| **Initialization:** $\theta \leftarrow \theta_0$, $t \leftarrow 1$; |
| **for** $1 \leq t \leq T$ **do** |
| $m \leftarrow \max\{C \times M, 1\}$; |
| RW $\leftarrow$ (random set of $m$ workers); |
| Multicast $\theta_{t-1}$ to workers in RW; |
| Wait to receive $\theta_{i,t}$ for $i \in$ RW; |
| $\theta_t \leftarrow \sum_{i \in \text{RW}} \frac{n_i}{\sum_{i \in S} n_i} \theta_{i,t}$; |
| $t + +$; |
| **return** $\theta_T$; |
For each round $t$, the local program at each recruited worker $i$ has the following inputs: $s$ – the number of local iterations; $B$ – the minibath size; $\eta$ – the stepsize; $\theta_{t-1}$. The first three are a priori inputs, and last one is received from the parameter server in each participating round.

**FedLWorker 2: FedAvg** Recruited worker $i$ of round $t$

1. **Input:** $B, s, \eta, \theta_{t-1};$
2. **Output:** $\theta_{i,t};$

3. **Initialization:** $r \leftarrow 1;$
4. $\theta_i \leftarrow \theta_{t-1}; \mathcal{B} \leftarrow \text{partition } S_i \text{ into batches of size } B;$
5. for $1 \leq r \leq s$ do
6.   for $b \in \mathcal{B}$ do
7.     $\theta_i \leftarrow \theta_i - \eta \nabla L_i(\theta_i ; b);$  
8.     $r + +;$
9. $\theta_{i,t} \leftarrow \theta_i;$
10. **return** $\theta_{i,t};$

**A.2 FedProx** [LSZ+18]

FedProx is a proximal variant of FedAvg wherein, instead of performing multiple local gradient descent updates, a participating worker uses a proximal update which involves solving a minimization problem. In practice, as minimization might not be solved exactly, a notion of $\gamma$-inexact minimizer is introduced [LSZ+18]. For each worker $i$, $(\gamma_{i,t}) \in \mathbb{R}^\infty$ is a pre-specified sequence of inexactness.
In this section, we illustrate the impacts of using minibatch on the achievability of stationary points and on the estimation errors of FedAvg and FedProx. For linear models, the minimization problems in FedLWorker 4 have closed form solutions. Thus, in our experiments, the local minimization problems are solved exactly. We consider the same setup used in Fig.1. Recall that \( n_i = 500 \), i.e., each worker keeps 500 data tuples. We run experiments with three batch sizes \( B \): 20, 50, and 100.

As formally described in FedLWorker 2: each worker \( i \) first partitions its local data into batches of the chosen size \( B \) (line 4 of the pseudocode), and then for each of the \( s \) local steps (each iteration of the outer for-loop from line 5 to line 8), worker \( i \) updates \( \theta_i \) via running gradient descent \( n_i B \) times, where a different batch in the data partition is used each time (the inner for-loop from line 6 to line 7). In this way, each of the batches is passed \( s \) times in a participating round. Recall that in Fig.1a and Fig.1b a full pass of local data \( S_i \) is used in each of the gradient descent update. For ease of comparison, we redraw Fig.1a and Fig.1b in Fig.5a and Fig.6a, respectively.

As illustrated in Figure 5, for \( s = 5 \) and \( s = 10 \) the impacts of different batch sizes on the gradient magnitude are negligible. However, strikingly, for FedAvg \( s = 1 \) with minibatch, its gradient magnitude rises up significantly and hence it can no longer reach the stationary point (This can be rigorously proved by following the arguments in [PW20]). For FedProx with minibatch, its curve mostly coincides with that of FedAvg \( s = 1 \).

In contrast, as shown in Fig.6, the minibatch has almost no effect on the estimation error. The final estimation errors are almost identical in each of the four figures in Fig.6. The convergence speed of FedAvg \( s = 1 \) only decreases a bit with minibatch.
In conclusion, we see that both FedAvg and FedProx with minibatch can converge to the optimal estimation error despite the unreachability of the stationary points.

C Preliminaries: Reproducing Kernel Hilbert Spaces

We present a brief overview of the key notion and results on reproducing kernels that are used in this paper. Interested readers are referred to [Wai19] for a detailed exploration on this topic. Any symmetric and positive semi-definite kernel function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ defines a reproducing kernel Hilbert space (RKHS) [Wai19, Theorem 12.11]. Let $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ denote the inner product of the RKHS such that $k(\cdot, x)$ acts as the representer of evaluation, i.e., $\langle f, k(x, \cdot) \rangle_{\mathcal{H}} = f(x)$ for $f \in \mathcal{H}$. Let $\|g\|_{\mathcal{H}} = \sqrt{\langle g, g \rangle_{\mathcal{H}}}$ denote the norm of function $g$ in the RKHS $\mathcal{H}$. For a given distribution $\mathbb{P}$ on $\mathcal{X}$, let $\|g\|_{2} = (\int_{\mathcal{X}} g(x)^{2}d\mathbb{P}(x))^{1/2}$ denote the norm in $L^{2}(\mathbb{P})$. In this paper, we take the following minimal assumptions that are common in literature [Wai19]: We assume that $\mathcal{X}$ is compact, $k$ is continuous, $\sup_{x \in \mathcal{X}} k(x, x) < \infty$, and that $\int_{\mathcal{X} \times \mathcal{X}} k^{2}(x, z)d\mathbb{P}(x)d\mathbb{P}(z) < \infty$. Let the Mercer expansion
Define the feature mapping $\phi : X \to \ell^2(N)$ as

$$\phi(x) = [\sqrt{\mu_1} \varphi_1(x), \sqrt{\mu_2} \varphi_2(x), \ldots]$$

where $\ell^2(N)$ denotes the space of square-summable sequences. Then for any $f \in \mathcal{H}$ with $f = \sum_{\ell=1}^{\infty} \beta_{\ell} \varphi_{\ell} = \langle \phi(x), \theta \rangle$, the following is true:

$$\|f\|_2^2 = \int_X f^2(x) d\mathbb{P} = \sum_{\ell=1}^{\infty} \beta_{\ell}^2,$$

and

$$\|f\|_{H}^2 = \sum_{\ell=1}^{\infty} \frac{\beta_{\ell}^2}{\mu_{\ell}} = \sum_{\ell=1}^{\infty} \theta_{\ell}^2.$$
D  Missing proofs of results in Section 3

D.1  Proof of Proposition 1

For FedAvg, recall that $\theta_{i,t} = P_i^s(\theta_{t-1})$, where $P_i(\theta) = \theta - \eta_i \nabla L_i(\theta)$ is the mapping of one-step local gradient descent, and $L_i(\theta) = \frac{1}{2} \|\phi(X_i)\theta - y_i\|^2$. Hence,

$$P_i(\theta) = \theta - \eta_i \left[ \phi(X_i)^\top (\phi(X_i)\theta - y_i) \right] = \left[ I - \eta_i \phi(X_i)^\top \phi(X_i) \right] \theta + \eta_i \phi(X_i)^\top y_i.$$ 

Iteratively applying $s$ times the mapping $P_i$, we get

$$P_i^s(\theta) = \left[ I - \eta_i \phi(X_i)^\top \phi(X_i) \right] \theta + \sum_{t=0}^{s-1} \left[ I - \eta_i \phi(X_i)^\top \phi(X_i) \right] \eta_i \phi(X_i)^\top y_i.$$ 

Combining the last display with (3) yields that

$$\theta_t = \sum_{i=1}^M w_i \left[ I - \eta_i \phi(X_i)^\top \phi(X_i) \right] \theta_{t-1} + \sum_{i=1}^M w_i \sum_{t=0}^{s-1} \left[ I - \eta_i \phi(X_i)^\top \phi(X_i) \right] \eta_i \phi(X_i)^\top y_i$$

$$= A\theta_{t-1} + By,$$

proving (8) for FedAvg. For FedProx, it follows from (2) that

$$\theta_{i,t} = \arg\min_{\theta} \frac{1}{2} \|\phi(X_i)\theta - y_i\|^2 + \frac{1}{2\eta_i} \|\theta - \theta_{t-1}\|^2$$

$$= \left[ I + \eta_i \phi(X_i)^\top \phi(X_i) \right]^{-1} \left( \theta_{t-1} + \eta_i \phi(X_i)^\top y_i \right).$$

Combining the last display with (3) yields that

$$\theta_t = \sum_{i=1}^M w_i \left[ I + \eta_i \phi(X_i)^\top \phi(X_i) \right]^{-1} \theta_{t-1} + \sum_{i=1}^M w_i \left[ I + \eta_i \phi(X_i)^\top \phi(X_i) \right]^{-1} \eta_i \phi(X_i)^\top y_i$$

$$= A\theta_{t-1} + By,$$

proving (8) for FedProx.

Next we show (10). Recall that $y = [y_1^\top, \ldots, y_M^\top]^\top$, where

$$y_i = \phi(X_i)\theta^*_i + \xi_i = \phi(X_i)\theta^* + \xi_i + \phi(X_i)(\theta^*_i - \theta^*).$$

Then we have

$$By = B\phi(X)\theta^* + B\xi + B\Delta_{\theta^*} = (I - A)\theta^* + B\xi + B\Delta_{\theta^*},$$

where we used the identity $B\phi(X) = I - A$ stated in Lemma 1. Subtracting both sides of (8) by $\theta^*$ and plugging in the last display, we get

$$\theta_t - \theta^* = A\theta_{t-1} - A\theta^* + B\xi + B\Delta_{\theta^*},$$

proving (10).
D.2 Proof of Proposition 2

Note that \( \vec{f}_t = \phi(X)\theta_t \). It follows from (8) that
\[
\vec{f}_t = \phi(X)\theta_t = \phi(X)(A\theta_{t-1} + By).
\]

From Lemma 1 we have
\[
\phi(X)A = (I - \eta KP) \phi(X), \text{ and } \phi(X)B = \eta KP.
\]

Thus,
\[
\vec{f}_t = \phi(X)(A\theta_{t-1} + By) = (I - \eta KP) \phi(X)\theta_{t-1} + \eta KP y
\]
\[
= (I - \eta KP) \vec{f}_{t-1} + \eta KP y,
\]
proving (13). Subtracting both sides of (13) by \( \vec{f}^* \), we get
\[
\vec{f}_t - \vec{f}^* = [I - \eta KP] \vec{f}_{t-1} + \eta KP y - \vec{f}^*
\]
\[
= [I - \eta KP] \left( \vec{f}_{t-1} - \vec{f}^* \right) + \eta KP \xi + \eta KP \begin{bmatrix}
\vec{f}^*_1(X_1) \\
\vdots \\
\vec{f}^*_M(X_M)
\end{bmatrix} - \eta KP \vec{f}^*
\]
\[
= [I - \eta KP] \left( \vec{f}_{t-1} - \vec{f}^* \right) + \eta KP \xi + \eta KP \Delta_{f^*},
\]
proving (14).

D.3 Proof of Lemma 1

We first prove Lemma 1 for FedAvg. By the identity \( \sum_{\tau=0}^{t-1} (I - Z)^\tau Z = I - (I - Z)^t \), we get that
\[
\sum_{\ell=0}^{s-1} (I - \eta_i \phi(X_i)^\top \phi(X_i))^\ell \eta_i \phi(X_i)^\top \phi(X_i) = I - (I - \eta_i \phi(X_i)^\top \phi(X_i))^s.
\]

Hence, applying the definition of \( B \) in (7) yields that
\[
B\phi(X) = \sum_{i=1}^M w_i \sum_{\ell=0}^{s-1} (I - \eta_i \phi(X_i)^\top \phi(X_i))^\ell \eta_i \phi(X_i)^\top \phi(X_i)
\]
\[
= \sum_{i=1}^M w_i \left[ I - (I - \eta_i \phi(X_i)^\top \phi(X_i))^s \right] = I - A.
\]

Moreover, since
\[
\left( I - \eta_i \phi(X_i)^\top \phi(X_i) \right) \phi(X_i)^\top = \phi(X_i)^\top \left( I - \eta_i \phi(X_i) \phi(X_i)^\top \right),
\]
via induction it can be shown that
\[
(I - \eta_i \phi(X_i)^\top \phi(X_i))^\ell \phi(X_i)^\top = \phi(X_i)^\top (I - \eta_i \phi(X_i) \phi(X_i)^\top)^\ell, \quad \forall \ell.
\]
Recall that $w_i\eta_i = \eta/N$. Then,

\[ B = \left[ \begin{array}{c} w_1\eta_1 \sum_{\ell=0}^{s-1}(I - \eta_1\phi(X_1)^\top \phi(X_1))^\ell \phi(X_1)^\top, \ldots, w_M\eta_M \sum_{\ell=0}^{s-1}(I - \eta_M\phi(X_M)^\top \phi(X_M))^\ell \phi(X_M)^\top \end{array} \right] \]

\[ = \frac{\eta}{N} \left[ \begin{array}{c} \phi(X_1)^\top \sum_{\ell=0}^{s-1}(I - \eta_1\phi(X_1)^\top \phi(X_1))^\ell, \ldots, \phi(X_M)^\top \sum_{\ell=0}^{s-1}(I - \eta_M\phi(X_M)^\top \phi(X_M))^\ell \end{array} \right] \]

\[ = \frac{\eta}{N} \phi(X)^\top P. \]

Multiplying both sides by $\phi(X)$ on the left yields that

\[ \phi(X)B = \frac{\eta}{N} \phi(X)\phi(X)^\top P = \eta KP. \]

Further multiplying both sides by $\phi(X)$ on the right yields that

\[ \eta KP\phi(X) = \phi(X)B\phi(X) = \phi(X)(I - A). \]

Rearranging the terms, we get \[17\].

Analogously, for FedProx, by the identity $(I + Z)^{-1}Z = I - (I + Z)^{-1}$, we get that

\[ \left[ I + \eta_i\phi(X_i)^\top \phi(X_i) \right]^{-1} \eta_i\phi(X_i)^\top \phi(X_i) = I - \left[ I + \eta_i\phi(X_i)^\top \phi(X_i) \right]^{-1} \]

and hence

\[ B\phi(X) = \sum_{i=1}^{M} w_i \left[ I + \eta_i\phi(X_i)^\top \phi(X_i) \right]^{-1} \eta_i\phi(X_i)^\top \phi(X_i) \]

\[ = \sum_{i=1}^{M} w_i \left[ I - \left[ I + \eta_i\phi(X_i)^\top \phi(X_i) \right]^{-1} \right] = I - A. \]

In addition,

\[ \left[ I + \eta_i\phi(X_i)^\top \phi(X_i) \right]^{-1} \phi(X_i)^\top \]

\[ = \left[ I + \eta_i\phi(X_i)^\top \phi(X_i) \right]^{-1} \phi(X_i)^\top \left[ I + \eta_i\phi(X_i)\phi(X_i)^\top \right] \left[ I + \eta_i\phi(X_i)^\top \phi(X_i) \right]^{-1} \]

\[ = \left[ I + \eta_i\phi(X_i)^\top \phi(X_i) \right]^{-1} \left[ I + \eta_i\phi(X_i)\phi(X_i)^\top \phi(X_i) \right] \phi(X_i)^\top \left[ I + \eta_i\phi(X_i)^\top \phi(X_i) \right]^{-1} \]

\[ = \phi(X_i)^\top \left[ I + \eta_i\phi(X_i)\phi(X_i)^\top \right]^{-1}. \] \hspace{1cm} (35)

Thus

\[ B = \left[ w_1\eta_1 \left[ I + \eta_1\phi(X_1)^\top \phi(X_1) \right]^{-1} \phi(X_1)^\top, \ldots, w_M\eta_M \left[ I + \eta_M\phi(X_M)^\top \phi(X_M) \right]^{-1} \phi(X_M)^\top \right] \]

\[ = \frac{\eta}{N} \left[ \phi(X_1)^\top \left[ I + \eta_1\phi(X_1)\phi(X_1)^\top \right]^{-1}, \ldots, \phi(X_M)^\top \left[ I + \eta_M\phi(X_M)\phi(X_M)^\top \right]^{-1} \right] \]

\[ = \frac{\eta}{N} \phi(X)^\top P. \]

The rest of the proof is identical to that for FedAvg.

### E Missing proofs of results in Section 4

In this section, we present the missing proofs of results in Section 4. We focus on proving the results for FedAvg. The proof for FedProx follows verbatim using the facts that $\|P\|_2 \leq 1$ and that $\lambda_{\min}(P) \geq 1/\kappa$. 

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E.1 Proof of Theorem 1

We show the convergence of the prediction error in the $L^2(\mathbb{P}_N)$ norm, that is,

$$\|f_t - f^*\|_2^2 = \frac{1}{N} \|f_t - \bar{f}\|_2^2 = \frac{1}{N} \sum_{i=1}^{M} \sum_{j=1}^{n_i} (f_t(x_{ij}) - f^*(x_{ij}))^2.$$ 

Unrolling the recursion (15), we get

$$\vec{f}_t - \bar{f} = [I - \eta KP]^t (\vec{f}_0 - \bar{f}) + \sum_{\tau=0}^{t-1} [I - \eta KP]^\tau \eta KP (\xi + \Delta f^*)$$

(36) where the last equality follows from the identity that $\sum_{\tau=0}^{t-1} (I - A)^\tau A = I - (I - A)^t$. It follows that

$$\|\vec{f}_t - \bar{f}\|_2^2 \leq 3 \|I - \eta KP\|^t \|\bar{f}\|_2^2 + 3 \|I - [I - \eta KP]^t\| \|\xi\|_2^2 + 3 \|I - [I - \eta KP]^t\| \|\Delta f^*\|_2^2.$$ (37)

The following three lemmas respectively bound the first (bias), the second (variance), and third (model heterogeneity) terms in (37).

**Lemma 2 (Bias).** For all iterations $t = 1, 2, \ldots$, it holds that

$$\frac{1}{N} \|I - \eta KP\|^t \|\bar{f}\|_2^2 \leq \frac{\kappa}{2e\eta ts}.$$ 

**Lemma 3 (Variance).** For all iterations $t = 1, 2, \ldots$, it holds that

$$\frac{1}{N} \mathbb{E} \left[\|I - [I - \eta KP]^t\| \|\xi\|_2^2\right] \leq \kappa \sigma^2 \eta ts R_K^2 \left(\frac{1}{\sqrt{\eta ts}}\right).$$ (38)

Furthermore, if the coordinates of $\xi$ are $N$ independent zero-mean and sub-Gaussian variables (with sub-Gaussian norm $\sigma$), then there exists a universal constant $c_1$ such that for any $\delta > 0$,

$$\mathbb{P} \left\{ \frac{1}{N} \|I - [I - \eta KP]^t\| \|\xi\|_2^2 \leq \kappa \sigma^2 \eta ts R_K^2 \left(\frac{1}{\sqrt{\eta ts}}\right) + \frac{\delta}{N} \right\} \geq 1 - \exp \left( - \frac{c_1 \delta}{\sigma^2 \kappa} \right) \frac{\delta}{\sigma^2 \kappa N \eta ts R_K^2 \left(\frac{1}{\sqrt{\eta ts}}\right)}.$$ (39)

**Lemma 4 (Model heterogeneity).** For all iterations $t = 1, 2, \ldots$, it holds that

$$\frac{1}{N} \|I - [I - \eta KP]^t\| \|\Delta f^*\|_2^2 \leq \frac{\kappa}{N} \|\Delta f^*\|_2^2.$$ 

Finishing the proof of Theorem 1 Applying Lemmas 2 – 4 we get that

$$\mathbb{E} \left[\|f_t - f^*\|_2^2\right] \leq \frac{3\kappa}{2e\eta ts} + 3\kappa \sigma^2 \eta ts R_K^2 \left(\frac{1}{\sqrt{\eta ts}}\right) + \frac{3\kappa}{N} \|\Delta f^*\|_2^2 \leq \frac{3\kappa}{e\eta ts} + \frac{3\kappa}{N} \|\Delta f^*\|_2^2, \forall 1 \leq t \leq T,$$
where the last inequality holds by the early stopping rule (20); by the definition of $\epsilon_N$ in (19), we have $\epsilon_N^2 \leq \frac{1}{\eta Ts}$ and hence $\eta ts R_K(1/\sqrt{\eta Ts}) \leq 1/(\sqrt{2e}\sigma)$ follows from the fact that $R_K(\epsilon)/\epsilon^2$ is non-increasing in $\epsilon$.

Finally, by the definition of the critical radius $\epsilon_N$ in (19), we have $\epsilon_N^2 \geq \frac{1}{\eta(T+1)s}$ and hence

$$\eta ts R_K\left(\frac{1}{\sqrt{\eta Ts}}\right) \leq \frac{1}{\sqrt{2e}\sigma}$$

follows from the fact that $R_K(\epsilon)/\epsilon^2$ is non-increasing in $\epsilon$.

Moreover, under the additional sub-Gaussian assumption on $\xi$, applying (39) in Lemma 3 with $\delta = N\kappa/(\eta Ts)$, yields that for any $t \leq T$

$$\mathbb{P}\left\{ \frac{1}{N}\|I - [I - \eta KP]^t\|_2^2 \leq \kappa\sigma^2 \eta ts R_K^2 \left(\frac{1}{\sqrt{\eta Ts}}\right) + \frac{\kappa}{\eta Ts} \right\} \geq 1 - \exp\left( - \frac{c_1 N}{\sigma^2 \eta Ts} \min\left\{ 1, \frac{1}{\sigma^2 e(\eta Ts)^2 R_K^2 \left(\frac{1}{\sqrt{\eta Ts}}\right)} \right\} \right)$$

$$\geq 1 - \exp\left( - \frac{c_1 N}{\sigma^2 \eta Ts} \right)$$

$$\geq 1 - \exp\left( - \frac{c_1 N\epsilon_N^2}{\sigma^2} \right),$$

where the second-to-the-last inequality holds because $\eta ts R_K(1/\sqrt{\eta Ts}) \leq 1/(\sqrt{2e}\sigma)$, and the last inequality follows from $\eta Ts \leq \epsilon_N^{-2}$. Therefore, we get that

$$\|f_T - f^*\|_N^2 \leq \frac{12\kappa\epsilon_N^2}{e} + \frac{3\kappa}{N} \|\Delta f^*\|_2^2.$$  

E.1.1 Proof of Lemma 2

Our main idea is to apply the eigenvalue decomposition of $KP$ and to project $\tilde{f}^*$ to the eigenspace.

We first rewrite $[I - \eta KP]^t$ in terms of the eigenvalues and eigenvectors of $KP$. Recall from (4) that $\eta\|\phi(X_i)\|^2 \leq \gamma < 1$. By definition of (12), we know $P_{ii} > 0$, which implies that $P$ is positive-definite. Let $P^{1/2}$ denote the unique square root of $P$. Consider the symmetric matrix $P^{1/2}KP^{1/2}$ and denote its eigenvalue decomposition as

$$P^{1/2}KP^{1/2} = U\Lambda U^\top,$$  

where $UU^\top = U^\top U = I$, i.e., $U^\top = U^{-1}$, and $\Lambda$ is a $N \times N$ diagonal matrix with non-negative entries. We have

$$K = P^{-1/2}U\Lambda U^\top P^{-1/2} = V\Lambda V^\top,$$

$$KP = V\Lambda V^\top P = V\Lambda V^{-1},$$

where $V = P^{-1/2}U$ and $V^\top P = U^\top P^{1/2} = V^{-1}$. Consequently,

$$[I - \eta KP]^t = [VV^{-1} - \eta V\Lambda V^{-1}]^t = V[I - \eta\Lambda]^t V^{-1}. $$  

(41)
From (41) and the fact that $\bar{f}^* = \phi(X)\theta^*$, we have

$$
\left\| \left[ I - \eta KP \right]^t \bar{f}^* \right\|_2 = \left\| V \left[ I - \eta \Lambda \right]^t V^{-1} \phi(X)\theta^* \right\|_2 
\leq \left\| V \right\|_2 \left\| \left[ I - \eta \Lambda \right]^t V^{-1} \phi(X) \right\|_2 \left\| \theta^* \right\|_2. \tag{42}
$$

By the definition of $V$ and the block structure of $P$, we have

$$
\left\| V \right\|_2^2 = \left\| P^{-1} \right\|_2 = \max_{i \in [N]} \left\| P_{ii}^{-1} \right\|_2 = \max_{i \in [N]} \frac{1}{\lambda_{\min}(P_{ii})} \leq \frac{\gamma}{1 - (1 - \gamma)^s} = \kappa/s, \tag{43}
$$

where the inequality holds because by definition $\eta \left\| \phi(X_i) \right\|_2 \leq \gamma$ and the fact that $\frac{x}{1-(1-x)^s}$ is monotone increasing in $x \in [0,1]$. 

Note that $\left\| \left[ I - \eta \Lambda \right]^t V^{-1} \phi(X) \right\|_2 \leq \gamma$ and that $\gamma < 1$ by definition (6). Thus in view of Lemma 1,

$$
\frac{1}{N} \left\| \left[ I - \eta \Lambda \right]^t V^{-1} \phi(X) \right\|_2^2 = \left\| \left[ I - \eta \Lambda \right]^t V^{-1} K \left( V^{-1} \right)^\top \left[ I - \eta \Lambda \right]^t \right\|_2 
= \left\| \left[ I - \eta \Lambda \right]^t \Lambda \left[ I - \eta \Lambda \right]^t \right\|_2 
= \max_{j: 1 \leq j \leq N} (1 - \eta A_{jj})^2 \Lambda_{jj} 
\leq \frac{1}{2s}, \tag{44}
$$

where $\Lambda_{jj}$ is the $j$-th position in the diagonal of $\Lambda$, and the last inequality holds because that $(1 - x)^t x \leq \frac{1}{e^t}$ for all $x \leq 1$ and that $\eta A_{jj} \leq 1$ to be verified next. By (40), the condition $\eta A_{jj} \leq 1$ is equivalent to $\eta \left\| P^{1/2}K P^{1/2} \right\|_2 \leq 1$. Since $K = \frac{1}{N} \phi(X) \phi(X)^\top$ and $\left\| ZZ^\top \right\|_2 = \left\| Z^\top Z \right\|_2$, it follows that

$$
\eta \left\| P^{1/2}K P^{1/2} \right\|_2 = \left\| \frac{\eta}{N} \phi(X)^\top P\phi(X) \right\|_2. 
$$

Note that $\gamma < 1$ and hence $A \succeq 0$ by definition (6). Thus in view of Lemma 1,

$$
\frac{\eta}{N} \phi(X)^\top P\phi(X) = B\phi(X) = I - A \succeq I.
$$

The conclusion of Lemma 2 follows by applying (43), (44), and the assumption $\left\| \theta^* \right\|_2 = \left\| f^* \right\|_H \leq 1$ to (42).

**E.1.2 Proof of Lemma 3**

In this section, we bound the variance term. In view of the eigenvalue decomposition given in (41), we know

$$
\left[ I - \left[ I - \eta KP \right]^t \right] = V \left[ I - \left[ I - \eta \Lambda \right]^t \right] V^{-1}.
$$

Hence,

$$
\left\| V \left[ I - \left[ I - \eta \Lambda \right]^t \right] V^{-1} \xi \right\|_2^2 = \xi^\top Q \xi = \text{Tr} \left( \xi \xi^\top Q \right),
$$

where

$$
Q = \left( V^{-1} \right)^\top \left[ I - \left[ I - \eta \Lambda \right]^t \right] V^\top V \left[ I - \left[ I - \eta \Lambda \right]^t \right] V^{-1}. \tag{45}
$$

\(^1\)To see the monotonity, note that $\frac{1 - (1-x)^s}{x^s} = \sum_{t=0}^{s-1} (1-x)^t$, which is monotone decreasing in $x \in [0,1]$. 

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It is easy to see that $Q \succeq 0$ and by the assumption it holds that $\mathbb{E} [\xi \xi^T] \preceq \sigma^2 I$. Hence, using the fact that
\[
\text{Tr}(YZ) \geq 0, \quad \text{if } Y \succeq 0 \text{ and } Z \succeq 0,
\] (46)
we have
\[
\sigma^2 \text{Tr} (Q) - \mathbb{E} \left[ \text{Tr} \left( \xi \xi^T Q \right) \right] = \text{Tr} \left( \left( \sigma^2 I - \mathbb{E} [\xi \xi^T] \right) Q \right) \geq 0,
\] (47)
and hence
\[
\mathbb{E} \left[ \|V \left[ I - [I - \eta \Lambda]^t \right] V^{-1} \xi \|_2^2 \right] = \mathbb{E} \left[ \text{Tr} \left( \xi \xi^T Q \right) \right] \leq \sigma^2 \text{Tr}(Q).
\] (48)

Next we bound $\text{Tr}(Q)$. Similar to (47), since $V^{-1} (V^{-1})^T = U^T P U \preceq \|P\|_2 I$ and $V^T V = U^T P^{-1} U \preceq \|P^{-1}\|_2 I$, it follows that
\[
\text{Tr}(Q) \leq \|P\|_2 \|P^{-1}\|_2 \text{Tr} \left( \left[ I - [I - \eta \Lambda]^t \right]^2 \right) \leq \kappa \text{Tr} \left( \left[ I - [I - \eta \Lambda]^t \right]^2 \right),
\] (49)
where the last inequality holds because $\lambda_{\min}(P) \geq s/\kappa$ and $\|P\|_2 \leq s$. Recalling that $\Lambda_{ii}$ is the $i$-th diagonal entry in $\Lambda$ and that $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_N$ are the eigenvalues of $K$. It holds that
\[
\text{Tr} \left( \left[ I - [I - \eta \Lambda]^t \right]^2 \right) = \sum_{i=1}^{N} \left( 1 - (1 - \eta \Lambda_{ii})^t \right)^2
\]
\[
\leq \sum_{i=1}^{N} \min \left\{ 1, \eta^2 t^2 \Lambda_{ii}^2 \right\}
\]
\[
\leq \sum_{i=1}^{N} \min \left\{ 1, \eta t \Lambda_{ii} \right\}
\]
\[
\leq \sum_{i=1}^{N} \min \left\{ 1, \eta t \lambda_{is} \right\},
\]
where the last inequality holds because $\Lambda_{ii} \leq \lambda_i \|P\| \leq \lambda_i s$ in view of Ostrowski’s inequality (see e.g. [HJ12, Theorem 4.5.9]). It follows from the definition of $R_K$ in (18) that
\[
\frac{1}{N} \text{Tr} \left( \left[ I - [I - \eta \Lambda]^t \right]^2 \right) \leq \eta t s R_K^2 \left( \frac{1}{\sqrt{\eta t s}} \right).
\] (50)

We conclude (38) by combining (48) – (50).

It remains to prove the high-probability bound (39) under the additional sub-Gaussian assumption. Using Hanson-Wright’s inequality [RV+13], we get
\[
P \left\{ \left\langle \xi \xi^T, Q \right\rangle - \mathbb{E} \left[ \text{Tr} \left( \xi \xi^T Q \right) \right] \geq \delta \right\} \leq \exp \left( -c_1 \min \left\{ \frac{\delta}{\sigma^2 \|P\|_2^2}, \frac{\delta^2}{\sigma^4 \|P\|_F^2} \right\} \right),
\] (51)
where $c_1 > 0$ is a universal constant. Note that
\[
\|Q\|_2 \leq \|V^{-1}\|_2^2 \|V\|_2^2 = \|P\|_2 \|P^{-1}\|_2 \leq \kappa,
\] (52)
\[
\|Q\|_F^2 = \text{Tr}(QQ^T) \leq \|Q\|_2 \text{Tr}(Q),
\] (53)
where the last inequality follows from (46). Applying (49) – (50) yields that
\[ \frac{\delta^2}{\sigma^2 \|Q\|_F^2} \geq \frac{\delta}{\sigma^2 \|Q\|_2^2 \sigma^2 \text{Tr}(Q)} \geq \frac{\delta}{\sigma^2 \|Q\|_2^2 \sigma^2 \sigma N \eta \ell s K^2 \left( \frac{1}{\sqrt{q^2 s}} \right)} , \]
\[ \frac{\delta}{\sigma^2 \|Q\|_2^2} \geq \frac{\delta}{\sigma^2 \kappa} . \]

Thus we obtain that
\[ \min \left\{ \frac{\delta}{\sigma^2 \|Q\|_2^2}, \frac{\delta^2}{\sigma^4 \|Q\|_F^2} \right\} \geq \frac{\delta}{\sigma^2 \kappa} \min \left\{ 1, \frac{\delta}{\sigma^2 \kappa N \eta \ell s K^2 \left( \frac{1}{\sqrt{q^2 s}} \right)} \right\} . \]

The conclusion in (39) follows by combining (48), (51), and (54).

### E.1.3 Proof of Lemma 4

Note that
\[ \| (I - [I - \etaKP]^t) \Delta \|_2^2 \leq \| I - (I - \etaKP)^t \Delta \|_2^2 = \| Q \|_2 \| \Delta \|_2^2 . \]

From (52), we know the first term is at most $\kappa$. The proof is complete.

### E.2 Proof of Theorem 2

In this section, we show the convergence of the prediction error in the $L^2(\mathbb{P})$ norm. We focus on proving Theorem 2 for FedAvg – the proof for FedProx follows verbatim using $\|P\|_2 \leq 1$ and $\lambda_{\min}(P) \geq 1/\kappa$. The proof of Theorem 2 uses the following three auxiliary lemmas.

As a first step, we need to bound the RKHS norm of $f_t$, or equivalently the $\ell^2$ norm of $\theta_t$.

**Lemma 5.** There exists a universal constant $c_1$ such that for any $1 \leq t \leq T$, with probability at least $1 - \exp \left( -c_1 N \epsilon_N^2 / \sigma^2 \right)$, it holds that $\|f_t\|_{\mathcal{H}}^2 \leq 6 + \frac{3}{X_N} \| \Delta \|_2^2$.

Then we need to connect the prediction error in $L^2(\mathbb{P})$ norm and that in $L^2(\mathbb{P})$, and to connect the critical radius $\epsilon_N$ and $\bar{\epsilon}_N$, respectively. Towards this, we apply two well-known existing results, formally stated next.

**Lemma 6.** ([Wai19, Theorem 14.1.1]) Let $G$ denote the set of functions $g \in \mathcal{H}$ such that $\|g\|_{\infty} \leq B$ for constant $B$ and $\|g\|_{\mathcal{H}} \leq 1$. Then there exist universal constants $(c_1, c_2, c_3)$ such that for any $\delta \geq \bar{\epsilon}_N$, with probability at least $1 - c_1 \exp(-c_2 N \delta^2)$, it holds that
\[ \|g\|_2^2 \leq 2 \|g\|_{\mathcal{H}}^2 + c_3 \delta^2, \quad \forall g \in \mathcal{G} . \]

**Lemma 7.** ([Wai19, Proposition 14.25]) There exist constants $c_1, c_2, c_3, c_4$ such that with probability at least $1 - c_1 \exp(-c_2 N \epsilon_N^2)$, $c_3 \bar{\epsilon}_N \leq \epsilon_N \leq c_4 \bar{\epsilon}_N$.

Now we are ready to prove Theorem 2.

**Proof of Theorem 2.** It follows from Lemma 5 that with probability at least $1 - \exp \left( -c_1 N \epsilon_N^2 / \sigma^2 \right)$,$\|f_T\|_{\mathcal{H}}^2 \leq 6 + \frac{3}{X_N} \| \Delta \|_2^2$. Hence,
\[ \|f_T - f^*\|_{\mathcal{H}}^2 \leq 2 \|f^*\|_{\mathcal{H}}^2 + 2 \|f_T\|_{\mathcal{H}}^2 \leq 14 + \frac{6}{X_N} \| \Delta \|_2^2 , \]

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recalling that \( \|f^*\|_H^2 \leq 1 \). Applying Lemma 6 with \( g = \frac{f_t - f^*}{\|f_t - f^*\|_H} \) and \( \delta = \bar{\epsilon}_N \), Theorem 1 and Lemma 7, we get that with probability at least \( 1 - c_1 \exp(-c_2 N \bar{\epsilon}_N^2) \),

\[
\|f_T - f^*\|_2^2 \leq c_3 \kappa \left( \bar{\epsilon}_N^2 + \|\Delta \theta^*\|_2^2 / N \right). 
\]

By integrating out the tail probability, we can further get that

\[
\mathbb{E}_{X, \xi} \left[ \|f_T - f^*\|_2^2 \right] \leq c_4 \kappa \left( \bar{\epsilon}_N^2 + \|\Delta \theta^*\|_2^2 / N \right). 
\]

---

**E.2.1 Proof of Lemma 5**

Since \( \|f_t\|_H = \|\theta_t\|_2 \), it is equivalent to bound \( \|\theta_t\|_2 \). Recall the definitions of \( A \) and \( B \) for FedAvg in (6) and (7), respectively. It follows from Proposition 1 and \( \theta_0 = 0 \) that

\[
\theta_t = (I - A^t) \theta^* + \sum_{\tau=0}^{t-1} A^\tau B (\xi + \Delta \theta^*). 
\]

Note that \( A \succeq 0 \) and \( \|A\|_2 \leq 1 \). Thus,

\[
\|\theta_t\|_2^2 \leq 3 \|\theta^*\|_2^2 + 3 \left\| \sum_{\tau=0}^{t-1} A^\tau B \xi \right\|_2^2 + 3 \left\| \sum_{\tau=0}^{t-1} A^\tau B \Delta \theta^* \right\|_2^2. 
\]

Note that

\[
\left\| \sum_{\tau=0}^{t-1} A^\tau B \xi \right\|_2^2 \leq \text{Tr} \left( \xi^\top \tilde{Q} \right),
\]

where

\[
\tilde{Q} = B^\top \left( \sum_{\tau=0}^{t-1} A^\tau \right)^2 B.
\]

Moreover,

\[
\left\| \sum_{\tau=0}^{t-1} A^\tau B \Delta \theta^* \right\|_2^2 \leq \left( \sum_{\tau=0}^{t-1} A^\tau B \right)^2 \left\| \Delta \theta^* \right\|_2^2 \leq \|\tilde{Q}\|_2 \|\Delta \theta^*\|_2^2. 
\]

Therefore,

\[
\|\theta_t\|_2^2 \leq 3 \|\theta^*\|_2^2 + 3 \text{Tr} \left( \xi^\top \tilde{Q} \right) + 3 \|\tilde{Q}\|_2 \|\Delta \theta^*\|_2^2. 
\]

In view of (46), the fact that \( \tilde{Q} \succeq 0 \), and the assumption that \( \mathbb{E} \left[ \xi^\top \tilde{Q} \right] \leq \sigma^2 I \), we get that

\[
\mathbb{E} \left[ \text{Tr} \left( \xi^\top \tilde{Q} \right) \right] \leq \sigma^2 \text{Tr}(\tilde{Q}) = \sigma^2 \text{Tr} \left( B^\top \left( \sum_{\tau=0}^{t-1} A^\tau \right)^2 B \right) = \sigma^2 \text{Tr} \left( \left( \sum_{\tau=0}^{t-1} A^\tau \right)^2 BB^\top \right). 
\]

It follows from Lemma 1 and \( \|P\|_2 \leq s \) that

\[
BB^\top = \frac{\eta^2}{N^2} \phi^\top(X) P^2 \phi(X) \leq \frac{s \eta^2}{N^2} \phi^\top(X) P \phi(X) = \frac{s \eta}{N} B \phi(X) = \frac{s \eta}{N} (I - A). 
\]

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Hence we have
\[
\text{Tr}(\bar{Q}) \leq \frac{s\eta}{N} \text{Tr} \left( \left( \sum_{\tau=0}^{t-1} A^\tau \right)^2 (I - A) \right) = \frac{s\eta}{N} \text{Tr} \left( \sum_{\tau=0}^{t-1} A^\tau (I - A^\tau) \right). \tag{58}
\]

Let \( \lambda_1(A) \geq \lambda_2(A) \geq \cdots \) denote the eigenvalues of \( A \) in the non-increasing order. Applying the facts \( 1 - x^t \leq \min\{1, t(1 - x)\} \) and \( \min\{1, t^2x\} \leq \min\{t, t^2\} \) for \( t \geq 0 \) and \( 0 \leq x \leq 1 \), we obtain\n\[
\text{Tr} \left( \sum_{\tau=0}^{t-1} A^\tau (I - A^\tau) \right) = \sum_{i=1}^{\infty} \frac{(1 - \lambda_i(A))^2}{1 - \lambda_i(A)} \leq \sum_{i=1}^{\infty} \min \left\{ \frac{1}{1 - \lambda_i(A)}, t^2(1 - \lambda_i(A)) \right\} \leq \sum_{i=1}^{\infty} \min \left\{ t, t^2(1 - \lambda_i(A)) \right\}. \tag{59}
\]

Note that \( A \succeq I - \frac{s\eta}{N} \phi(X)^T \phi(X) \), and thus by Weyl’s inequality \( 1 - \lambda_i(A) \leq s\eta \lambda_i \) for \( 1 \leq i \leq N \) and \( 1 - \lambda_i(A) = 0 \) for \( i > N \). It follows that\n\[
\frac{1}{N} \text{Tr} \left( \sum_{\tau=0}^{t-1} A^\tau (I - A^\tau) \right) \leq \frac{1}{N} \sum_{i=1}^{N} \min \{ t, t^2 s\eta \lambda_i \} = t^2 s\eta R_K^2 \left( \frac{1}{\sqrt{\eta ts}} \right), \tag{60}
\]
where the last equality used the definition of \( R_K \) in \( \{15\} \). Recall \( T \) from the early stopping rule \( \{20\} \), it holds that \( \eta ts R_K (1/\sqrt{\eta ts}) \leq 1/(\sqrt{2\sigma}) \) for \( t \leq T \). Therefore, by \( \{56\}, \{58\}, \) and \( \{60\} \), for \( t \leq T \),
\[
E[\text{Tr} \left( \xi \xi^T \bar{Q} \right)] \leq \sigma^2 \text{Tr}(\bar{Q}) \leq \left( \sigma s\eta R_K \left( \frac{1}{\sqrt{\eta ts}} \right) \right)^2 \leq \frac{1}{2e}. \tag{61}
\]

Moreover,
\[
\|\bar{Q}\|_2 = \left\| \left( \sum_{\tau=0}^{t-1} A^\tau \right) BB^T \left( \sum_{\tau=0}^{t-1} A^\tau \right) \right\|_2 \geq \|Z^T Z\|_2 = \|ZZ^T\|_2 \leq \left\| \left( \sum_{\tau=0}^{t-1} A^\tau \right) \frac{s\eta}{N} (I - A) \left( \sum_{\tau=0}^{t-1} A^\tau \right) \right\|_2 \leq \left\| \left( \sum_{\tau=0}^{t-1} A^\tau (I - A^\tau) \right) \right\|_2 \leq \frac{\eta ts}{N}. \tag{62}
\]

It remains to derive the high-probability bound. Using the Hanson-Wright inequality \( \{RV+13\} \),
\[
P \left\{ \left( \xi \xi^T, \bar{Q} \right) - E \left[ \left( \xi \xi^T, \bar{Q} \right) \right] \geq \delta \right\} \leq \exp \left( -c_1 \min \left\{ \frac{\delta}{\sigma^2 \|\bar{Q}\|_2}, \frac{\delta^2}{\sigma^4 \|\bar{Q}\|_2^2} \right\} \right),
\]
where \( c_1 > 0 \) is a universal constant.

Since \( \bar{Q} \succeq 0 \), \( \|\bar{Q}\|_2 \leq \|\bar{Q}\|_2 \) \( \text{Tr}(\bar{Q}) \). Choosing \( \delta = \frac{1}{2e} \) and invoking \( \sigma^2 \text{Tr}(\bar{Q}) \leq \delta \) from \( \{61\} \), we get that\n\[
P \left\{ \left( \xi \xi^T, \bar{Q} \right) - E \left[ \left( \xi \xi^T, \bar{Q} \right) \right] \geq \delta \right\} \leq \exp \left( -c_1 \min \left\{ \frac{N}{2\sigma^2 e\eta ts}, \frac{N}{2\sigma^2 e} \right\} \right) = \exp \left( -c_1 N e^2 / (2\sigma^2 e) \right), \tag{63}
\]

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where the last inequality holds because \( \eta ts \leq \epsilon_N^{-2} \) for all \( 1 \leq t \leq T \). Hence, combining (55), (61), (62), (63), and the assumption \( \|\theta^*\|_2 = \|f^*\|_{\mathcal{H}} \leq 1 \), with probability at least \( 1 - \exp(-c_1N\epsilon_N^2/(2\sigma^2)) \),

\[
\|\theta_t\|_2^2 \leq 3 + 3/e + 3\frac{\eta ts}{N}\|\Delta_{\theta^*}\|_2^2 \leq 6 + 3\frac{\epsilon_N}{N}\|\Delta_{\theta^*}\|_2^2 ,
\]

where the last inequality follows from \( \eta ts \leq \epsilon_N^{-2} \) for all \( 1 \leq t \leq T \).

### E.2.2 Proof of Corollary 1
Since the kernel \( k \) has finite rank \( r \), we have \( \lambda_i = 0 \) for all \( i > r \) and hence

\[
\bar{R}_k(\epsilon) = \sqrt{\frac{1}{N}\sum_{i=1}^{\infty}\min\{\lambda_i, \epsilon^2\}} = \sqrt{\frac{1}{N}\sum_{i=1}^{r}\min\{\lambda_i, \epsilon^2\}} \leq \sqrt{\frac{r}{N}}\epsilon .
\]

Therefore, by the definition of \( \bar{\epsilon}_N \), we get that

\[
\frac{\bar{\epsilon}_N^2}{2\sigma} = \bar{R}_k(\epsilon_N) \leq \sqrt{\frac{r}{N}}\bar{\epsilon}_N ,
\]

and hence

\[
\bar{\epsilon}_N \leq 2\sigma\sqrt{\frac{r}{N}},
\]

which completes the proof in view of Theorem 2.

### E.2.3 Proof of Corollary 2
Since the kernel \( k \) satisfies the eigenvalue decay (22), we have

\[
\tilde{R}_k(\epsilon) \leq \sqrt{\frac{1}{N}\sum_{i=1}^{\infty}\min\{C_i^{-1}2, \epsilon^2\}} \leq \frac{C'}{\sqrt{N}}\epsilon^{1-1/(2\beta)} ,
\]

where the last inequality follows from [RWY14, Corollary 3]. Therefore, by the definition of \( \bar{\epsilon}_N \), we get that

\[
\frac{\bar{\epsilon}_N^2}{2\sigma} = \tilde{R}_k(\epsilon_N) \leq \frac{C'}{\sqrt{N}}\epsilon_N^{1-1/(2\beta)} ,
\]

and hence

\[
\bar{\epsilon}_N \leq \left(\frac{2\sigma C'}{\sqrt{N}}\right)^{2\beta/(2\beta+1)} ,
\]

which completes the proof in view of Theorem 2.

### E.3 Proof of Theorem 3
We first show this theorem for FedAvg. By the definition of \( \kappa \) in (5), we can show the following:

\[
\left(I - \eta_i\phi(X_i)\phi(X_i)^\top\right)^s \preceq I - (s/\kappa)\eta_i\phi(X_i)\phi(X_i)^\top .
\]
To see this, denote the eigenvalue decomposition of $\eta_i \phi(X_i)^T \phi(X_i)$ by $W \Sigma W^T$, where $W^T W = WW^T = I$. Then
\[
\left( I - \eta_i \phi(X_i)^T \phi(X_i) \right)^s = W (I - \Sigma)^s W^T \quad \text{and} \quad I - (s/\kappa) \eta_i \phi(X_i)^T \phi(X_i) = W (I - (s/\kappa) \Sigma) W^T.
\]
Hence, it suffices to check that $(1 - \Sigma_{ii})^s \leq 1 - (s/\kappa) \Sigma_{ii}$, or equivalently, $\kappa \geq \frac{s \Sigma_{ii}}{1 - (1 - \gamma) \kappa}$. Recall that by definition of $\gamma$ and $\kappa$, we have $0 \leq \Sigma_{ii} \leq \gamma \leq 1$ and $\kappa = \frac{\gamma \kappa}{1 - (1 - \gamma) \kappa}$. Thus we get $\kappa \geq \frac{s \Sigma_{ii}}{1 - (1 - \gamma) \kappa}$, as $\frac{x}{1 - (1 - x)^\gamma}$ is monotone increasing in $x \in [0, 1]$ (see the footnote [1]). From (64), it holds that
\[
A \leq I - (s/\kappa) \eta \frac{1}{N} \phi(X)^T \phi(X).
\]
Recall that $\rho = \lambda_{\min}(\phi(X)^T \phi(X)/N) > 0$. Thus $I - A \succeq (s/\kappa) \eta \rho I$ and $\|A\|_2 \leq 1 - (s/\kappa) \eta \rho$. In view of Lemma[1] $B \phi(X) = I - A$ and thus $B \Delta \theta^* = 0$ according to (9). It follows from Proposition[1] that
\[
\theta_t - \theta^* = -A^t \theta^* + \sum_{\tau=0}^{t-1} A^\tau B \xi.
\]
Since $\|A\|_2 \leq 1 - s \eta \rho / \kappa$, we have
\[
A^t \preceq \left( 1 - \frac{s \eta \rho}{\kappa} \right)^t I.
\]
Therefore,
\[
E \left[ \|\theta_t - \theta^*\|_2^2 \right] \leq \left( 1 - \frac{s \eta \rho}{\kappa} \right)^{2t} \|\theta^*\|_2^2 + E \left[ \left\| \sum_{\tau=0}^{t-1} A^\tau B \xi \right\|_2^2 \right].
\]
Moreover, since $A \in \mathbb{R}^{d \times d}$, combining (58) and (59) yields that
\[
E \left[ \left\| \sum_{\tau=0}^{t-1} A^\tau B \xi \right\|_2^2 \right] \leq \sigma^2 s \eta \frac{1}{N} \sum_{i=1}^d \frac{1}{1 - \lambda_i(A)} \leq \sigma^2 s \frac{\eta d}{N s \eta \rho / \kappa} = \sigma^2 \kappa \frac{d}{N \rho}.
\]
Combining the last two displayed equations yields the desired (24). It remains to establish (26). Using the fact that $B \phi(X) = I - A$, we have
\[
\theta^* - \theta_j^* = (I - A)^{-1} B \begin{bmatrix} \phi(X_1)(\theta_1^* - \theta_j^*) \\ \vdots \\ \phi(X_M)(\theta_M^* - \theta_j^*) \end{bmatrix}.
\]
We obtain from (57) that
\[
\left\| (I - A)^{-1} B \right\|_2^2 = \left\| (I - A)^{-1} BB^T (I - A)^{-1} \right\|_2 \leq \frac{s \eta}{N} \| (I - A)^{-1} \|_2 \leq \frac{\kappa}{N \rho},
\]
where we used $\lambda_{\min}(I - A) \succeq (s/\kappa) \eta \rho$. Consequently, since $\|\theta_t - \theta_j\|_2 \leq \Delta$, we get that
\[
\|\theta^* - \theta_j^*\|_2 \leq \left\| (I - A)^{-1} B \right\|_2 \left( \sum_{i=1}^M \|\phi(X_i)(\theta_i^* - \theta_j^*)\|_2^2 \right)^{1/2} \leq \Delta \sqrt{\frac{\kappa}{N \rho} \sum_{i=1}^M \|\phi(X_i)\|_2^2}.
\]
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E.4 Proof of Corollary 3

In view of [Ver10, Theorem 5.39] and the union bound, with probability at least $1 - e^{-d}$,

$$\sigma_{\min}(\phi(X)) \geq \sqrt{N} - c_1 \sqrt{d}, \quad \|\phi(X)\|_2 \leq \sqrt{N} + c_1 \sqrt{d},$$

and

$$\|\phi(X_i)\|_2 \leq \sqrt{n_i} + c_1 \sqrt{d} \quad \forall 1 \leq i \leq M,$$

where $\sigma_{\min}$ denotes the minimum singular value, and $c_1$ is a universal constant, and the last displayed equation holds under the additional assumption that $d \geq \log M$. Therefore, if $N \geq Cd$, then $\sigma_{\min}(\phi(X)) \geq \sqrt{N}/2$ and hence $\rho \geq 1/2$. Thus choosing $\eta \leq c_2 \min\{1, n_i/d\}$ for some sufficiently small constant $c_2$, we have that $c < 1$. Thus the desired conclusion (27) readily follows from Theorem 3.

It remains to prove (28). It follows from the last displayed equation that

$$\frac{M}{N} \sum_{i=1}^{M} \|\phi(X_i)\|_2^2 \leq \sum_{i=1}^{M} \left( \sqrt{n_i} + c_1 \sqrt{d} \right)^2 \leq 2 \sum_{i=1}^{M} \left( n_i + c_1^2 d \right) = 2N + 2c_1^2 Md.$$

It follows from (26) that

$$\|\theta^* - \theta_j\|_2 \leq \Delta \sqrt{\frac{\kappa}{N/2}} \sqrt{2N + 2c_1^2 Md} \leq c_3 \Delta \sqrt{\kappa} \left( 1 + \sqrt{\frac{Md}{N}} \right),$$

for a universal constant $c_3 > 0$.

E.5 Proof of Corollary 4

Note that

$$\frac{1}{N} \phi(X)^\top \phi(X) = \frac{1}{N} \sum_{i=1}^{M} \phi^\top(X_i) \phi(X_i) = \frac{1}{N} \sum_{i=1}^{M} U_i F_i^\top F_i U_i^\top \geq \alpha \sum_{i=1}^{M} w_i \frac{d}{r_i} U_i U_i^\top. \quad (65)$$

Note that $\mathbb{E} \left[ U_i U_i^\top \right] = \frac{\nu_d}{d} I_d$. Thus,

$$\sum_{i=1}^{M} w_i \frac{d}{r_i} \mathbb{E} \left[ U_i U_i^\top \right] = I_d, \quad (66)$$

Let

$$Y_i = w_i \frac{d}{r_i} \left[ U_i U_i^\top \mathbb{E} \left[ U_i U_i^\top \right] \right].$$
Let us use the matrix Bernstein inequality to bound the deviation of \( \sum_{i=1}^{M} Y_i \). Note that \( \|Y_i\|_2 \leq 2w_i d/r_i \) and

\[
\left\| \sum_{i=1}^{M} \mathbb{E}[Y_i^2] \right\|_2 = \left\| \sum_{i=1}^{M} w_i^2 \frac{d^2}{r_i^2} \left( \mathbb{E}[U_i U_i^\top] - \left( \mathbb{E}[U_i U_i^\top] \right) \right)^2 \right\|_2 \\
= \left\| \sum_{i=1}^{M} w_i^2 \frac{d^2}{r_i^2} \left( \frac{r_i}{d} I_d - \left( \frac{r_i}{d} \right)^2 I_d \right) \right\|_2 \\
\leq \sum_{i=1}^{M} w_i^2 \frac{d}{r_i}.
\]

Therefore, by the matrix Bernstein inequality, with probability at least \( 1 - d^{-1} \), for a universal constant \( c_3 > 0 \),

\[
\left\| \sum_{i=1}^{M} Y_i \right\|_2 \leq c_3 \sqrt{\sum_{i=1}^{M} w_i^2 \frac{d}{r_i} \log d + c_3 \max_{1 \leq i \leq M} w_i \frac{d}{r_i} \log d} \\
\overset{(a)}{\leq} c_3 \sqrt{\frac{\gamma d \log d}{N} + c_3 \frac{\gamma d \log d}{N}} \\
\overset{(b)}{\leq} \frac{1}{2},
\]

(67)

where (a) holds by definition \( \gamma = \max_{1 \leq i \leq M} n_i / r_i \) and \( w_i = n_i / N \); (b) holds by the assumption that \( N \geq C \gamma d \log d \) for a sufficiently large constant \( C \). Therefore, combining (66) and (67),

\[
\frac{1}{N} \phi(X)^\top \phi(X) \geq \alpha \sum_{i=1}^{M} w_i \frac{d}{r_i} U_i U_i^\top \geq \frac{\alpha}{2} I_d.
\]

Finally, since \( \|\phi(X)\|_2 = \|F_i\|_2 \). By choosing \( \eta \leq \min_{i \in [M]} \frac{n_i}{\|F_i\|^2} \), we have that \( \eta < 1 \). Thus the desired conclusion (31) readily follows from Theorem 3.

It remains to prove (32) using (26) in Theorem 3. Analogous to the last displayed equation, we have

\[
\frac{1}{N} \phi(X)^\top \phi(X) \leq \beta \sum_{i=1}^{M} w_i \frac{d}{r_i} U_i U_i^\top \leq \frac{3}{2} \beta.
\]

(68)

Thus, \( \|\phi(X)\|_2 \leq \sqrt{\frac{3\beta N}{2}} \). Moreover,

\[
\sum_{i=1}^{M} \|\phi(X_i)\|_2^2 \leq \sum_{i=1}^{M} \|\Sigma_i\|_2^2 \leq \beta d \sum_{i=1}^{M} \frac{n_i}{r_i} \leq \beta \gamma M d.
\]

It follows from (26) that

\[
\|\theta^* - \tilde{\theta}^*\|_2 \leq \Delta \sqrt{\frac{2\kappa \beta \gamma M d}{\alpha N}}.
\]