FedNEST: Federated Bilevel, Minimax, and Compositional Optimization

Davoud Ataee Tarzanagh 1  Mingchen Li 2  Christos Thrampoulidis 3  Samet Oymak 2

Abstract

Standard federated optimization methods successfully apply to stochastic problems with single-level structure. However, many contemporary ML problems – including adversarial robustness, hyperparameter tuning, actor-critic – fall under nested bilevel programming that subsumes minimax and compositional optimization. In this work, we propose FedNEST: A federated alternating stochastic gradient method to address general nested problems. We establish provable convergence rates for FedNEST in the presence of heterogeneous data and introduce variations for bilevel, minimax, and compositional optimization. FedNEST introduces multiple innovations including federated hypergradient computation and variance reduction to address inner-level heterogeneity. We complement our theory with experiments on hyperparameter & hyper-representation learning and minimax optimization that demonstrate the benefits of our method in practice.

1. Introduction

In the federated learning (FL) paradigm, multiple clients cooperate to learn a model under the orchestration of a central server (McMahan et al., 2017) without directly exchanging local client data with the server or other clients. The locality of data distinguishes FL from traditional distributed optimization and also motivates new methodologies to address heterogeneous data across clients. Additionally, cross-device FL across many edge devices presents additional challenges since only a small fraction of clients participate in each round, and clients cannot maintain state across rounds

1Email: tarzanaq@umich.edu, University of Michigan
2Emails: {ml11768, oymak@ece}ucr.edu, University of California, Riverside
3Email: cthrampo@ece.ubc.ca, University of British Columbia. Correspondence to: Davoud Ataee Tarzanagh <tarzanaq@umich.edu>.

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FL and incur high communication costs. To overcome this issue, popular FL methods, such as FEDAVG (McMahan et al., 2017), use local client updates, i.e. clients update their models multiple times before communicating with the server (aka, local SGD). Although FEDAVG has seen great success, recent works have exposed convergence issues in certain settings (Karimireddy et al., 2020; Hsu et al., 2019). This is due to a variety of factors, including client drift, where local models move away from globally optimal models due to objective and/or systems heterogeneity.

Existing FL methods, such as FEDAVG, are widely applied to stochastic problems with single-level structure. Instead, many machine learning tasks – such as adversarial learning (Madry et al., 2017), meta learning (Bertinetto et al., 2018), hyperparameter optimization (Franceschi et al., 2018), reinforcement/imitation learning (Wu et al., 2020; Arora et al., 2020), and neural architecture search (Liu et al., 2018) – admit nested formulations that go beyond the standard single-level structure. Towards addressing such nested problems, bilevel optimization has received significant attention in the recent literature (Ghadimi & Wang, 2018; Hong et al., 2020; Ji et al., 2021); albeit in non-FL settings. On the other hand, federated versions have been elusive perhaps due to the additional challenges surrounding heterogeneity, communication, and inverse Hessian approximation.

Contributions: This paper addresses these challenges and develops FedNEST: A federated machinery for nested problems with provable convergence and lightweight communication. FedNEST is composed of FedINN: a federated stochastic variance reduction algorithm (FedSVRG) to solve the inner problem while avoiding client drift, and FedOUT: a communication-efficient federated hypergradient algorithm for solving the outer problem. Importantly, we allow both inner & outer objectives to be finite sums over heterogeneous client functions. FedNEST runs a variant of FedSVRG on inner & outer variables in an alternating fashion as outlined in Algorithm 1. We make multiple algorithmic and theoretical contributions summarized below.

- The variance reduction of FedINN enables robustness in the sense that local models converge to the globally optimal inner model despite client drift/heterogeneity unlike FEDAVG. While FedINN is similar to FedSVRG (Konečný et al., 2018) and FedLin (Mitra et al., 2021), we make two key contributions: (i) We
leverage the global convergence of FEDINN to ensure accurate hypergradient computation which is crucial for our bilevel proof. (ii) We establish new convergence guarantees for single-level stochastic non-convex FEDSVRG, which are then integrated within our FEDOUT.

- **Communication efficient bilevel optimization**: Within FEDOUT, we develop an efficient federated method for hypergradient estimation that bypass Hessian computation. Our approach approximates the global Inverse Hessian-Gradient-Product (IHGP) via computation of matrix-vector products over few communication rounds.

- **LFEDNEST**: To further improve communication efficiency, we additionally propose a Light-FEDNEST algorithm, which computes hypergradients locally and only needs a single communication round for the outer update. Experiments reveal that LFEDNEST becomes very competitive as client functions become more homogeneous.

- **Unified federated nested theory**: We specialize our bilevel results to **minimax** and **compositional** optimization with emphasis on the former. For these, FEDNEST significantly simplifies and leads to faster convergence. Importantly, our results are on par with the state-of-the-art non-federated guarantees for nested optimization literature without additional assumptions (Table 1).

  We provide extensive **numerical experiments** \(^1\) on bilevel and minimax optimization problems. These demonstrate the benefits of FEDNEST, efficiency of LFEDNEST, and shed light on tradeoffs surrounding communication, computation, and heterogeneity.

### 2. Federated Nested Problems & FEDNEST

We will first provide the background on bilevel nested problems and then introduce our general federated method.

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\(^1\)FEDNEST code is available at [https://github.com/ucr-optml/FedNest](https://github.com/ucr-optml/FedNest).

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![Figure 1: Depiction of federated bilevel nested optimization and high-level summary of FEDNEST (Algorithm 1). At outer loop, FEDIHPG uses multiple rounds of matrix-vector products to facilitate hypergradient computation while only communicating vectors. At inner loop, FEDINN uses FEDSVRG to avoid client drift and find the unique global minima. Both are crucial for establishing provable convergence of FEDNEST.](image)

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Table 1: Sample complexity of FEDNEST and comparable non-FL methods to find an \(\epsilon\)-stationary point of \(f\): \(\kappa_g := \ell_{g,1}/\mu_g\) and \(\kappa_f := \ell_{f,1}/\mu_f\). \(\kappa_g^g\) denotes a polynomial function of \(\kappa_g\). ALSET (Chen et al., 2021a), BSA (Ghadimi & Wang, 2018), TSSA (Hong et al., 2020), SGDA (Lin et al., 2020), SMD (Rafique et al., 2021), SCGD (Wang et al., 2017), and NASA (Ghadimi et al., 2020).

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#### 2.1. Preliminaries on Federated Nested Optimization

In federated bilevel learning, we consider the following nested optimization problem as depicted in Figure 1:

\[
\begin{align*}
&\min_{x \in \mathbb{R}^d_1} \quad f(x) = \frac{1}{m} \sum_{i=1}^m f_i(x, y^*(x)) \\
&\text{subject to} \quad y^*(x) \in \arg\min_{y \in \mathbb{R}^d_2} \frac{1}{m} \sum_{i=1}^m g_i(x, y) .
\end{align*}
\]
Algorithm 1 \textsc{FedNest}

1: Inputs: $K, T \in \mathbb{N}$; $(x^0, y^0) \in \mathbb{R}^{d_1+d_2}$; \textsc{FedINN},
2: \textsc{FedOUT} with stepsizes $((\alpha^k, \beta^k))_{k=0}^{K-1}$
3: for $k = 0, \ldots, K - 1$ do
4: \hspace{1em} $y^{k,0} = y^k$
5: for $t = 0, \ldots, T - 1$ do
6: \hspace{2em} $y^{k,t+1} = \textsc{FedINN} \left( y^k, y^{k,t}, \beta^k \right)$
7: \hspace{1em} $y^{k+1} = \textsc{FedOUT} \left( y^k, y^{k+1}, \alpha^k \right)$
8: end for
9: \hspace{1em} $x^{k+1} = \text{argmin}_{x \in \mathbb{R}^{d_2}} f(x)
10: end for

Recall that $m$ is the number of clients. Here, to model objective heterogeneity, each client $i$ is allowed to have its own individual outer & inner functions $(f_i, g_i)$. Moreover, we consider a general stochastic oracle model, access to local functions $(f_i, g_i)$ via stochastic sampling as follows:

\begin{align}
    f_i(x, y^*(x)) &:= \mathbb{E}_{\xi \sim \mathcal{C}_i} [ f_i(x, y^*(x); \xi) ], \\
    g_i(x, y) &:= \mathbb{E}_{\xi \sim \mathcal{D}_i} [ g_i(x, y; \xi) ],
\end{align}

(1b)

where $(\xi, \mathcal{C}, \mathcal{D})$ is the outer(inner) sampling distributions for the $i$th client. We emphasize that for $i \neq j$, the tuples $(f_i, g_i, \mathcal{C}_i, \mathcal{D}_i)$ can be different.

Example 1 (Hyperparameter tuning). Each client has local validation and training datasets associated with objectives $(f_i, g_i)$ corresponding to validation and training losses, respectively. The goal is finding hyper-parameters $x$ that lead to learning model parameters $y$ that minimize the (global) validation loss.

The stochastic bilevel problem (1) subsumes two popular problem classes with the nested structure: Stochastic MiniMax & Stochastic Compositional. Therefore, results on the general nested problem (1) also imply the results in these special cases. Below, we briefly describe them.

Minimax optimization. If $g_i(x, y; \xi) := -f_i(x, y; \xi)$ for all $i \in \mathcal{S}$, the stochastic bilevel problem (1) reduces to the stochastic minimax problem

$$
\min_{x \in \mathbb{R}^{d_1}} \max_{y \in \mathbb{R}^{d_2}} \frac{1}{m} \sum_{i=1}^{m} \mathbb{E} [ f_i(x, y; \xi) ].
$$

(2)

Motivated by applications in fair beamforming, training generative-adversarial networks (GANs) and robust machine learning, significant efforts have been made for solving (2) including (Daskalakis & Panageas, 2018; Gidel et al., 2018; Mokhtari et al., 2020; Thekumparampil et al., 2019).

Example 2 (GANs). We train a generative model $g_x(\cdot)$ and an adversarial model $a_y(\cdot)$ using client datasets $\mathcal{C}_i$. The local functions may for example take the form $f_i(x, y) = \mathbb{E}_{s \sim \mathcal{C}_i} \left[ \log a_y(s) \right] + \mathbb{E}_{z \sim \mathcal{D}_{s,w}} \left[ \log [1 - a_y(g_x(z))] \right]$.  

Compositional optimization. Suppose $f_i(x, y; \xi) := f_i(y; \xi)$ and $g_i$ is quadratic in $y$ given as $g_i(x, y; \xi) := \| y - r_i(x; \xi) \|^2$. Then, the bilevel problem (1) reduces to

$$
\min_{x \in \mathbb{R}^{d_1}} \max_{y \in \mathbb{R}^{d_2}} f(x) = \frac{1}{m} \sum_{i=1}^{m} f_i(y^*(x))
$$

subj. to $y^*(x) = \argmin_{y \in \mathbb{R}^{d_2}} \frac{1}{m} \sum_{i=1}^{m} g_i(x, y)$

(3)

with $f_i(y^*(x)) := \mathbb{E}_{\xi \sim \mathcal{C}_i} [ f_i(y^*(x); \xi) ]$ and $g_i(x, y) := \mathbb{E}_{\xi \sim \mathcal{D}_i} [ g_i(x, y; \xi) ]$. Optimization problems in the form of (3) occur for example in model agnostic meta-learning and policy evaluation in reinforcement learning (Finn et al., 2017; Ji et al., 2020b; Dai et al., 2017; Wang et al., 2017).

Assumptions. Let $z = (x, y) \in \mathbb{R}^{d_1+d_2}$. Throughout, we make the following assumptions on inner/outer objectives.

Assumption A (Well-behaved objectives). For all $i \in [m]$

(A1) $f_i(z), \nabla f_i(z), \nabla g_i(z), \nabla^2 g_i(z)$ are $\ell_{f_i}, \ell_{g_i}, \ell_{g_2}, \ell_{2}$-Lipschitz continuous, respectively; and

(A2) $g_i(x, y)$ is $\mu_g$-strongly convex in $y$ for all $x \in \mathbb{R}^{d_1}$.

Throughout, we use $\kappa_{g} = \ell_{g,1}/\mu_{g}$ to denote the condition number of the inner function $g$.

Assumption B (Stochastic samples). For all $i \in [m]$

(B1) $\nabla f_i(z; \xi), \nabla g_i(z; \xi), \nabla^2 g_i(z; \xi)$ are unbiased estimators of $\nabla f_i(z), \nabla g_i(z), \nabla^2 g_i(z)$, respectively; and

(B2) Their variances are bounded, i.e., $\mathbb{E}_{\xi} [ \| \nabla f_i(z; \xi) - \nabla f_i(z) \|^2 ] \leq \sigma^2_{f_i}$, $\mathbb{E}_{\xi} [ \| \nabla^2 g_i(z; \xi) - \nabla^2 g_i(z) \|^2 ] \leq \sigma^2_{g_2}$, and $\mathbb{E}_{\xi} [ \| \nabla^2 g_i(z; \xi) - \nabla^2 g_i(z) \|^2 ] \leq \sigma^2_{g,2}$ for some $\sigma^2_{f_i}, \sigma^2_{g_2}, \sigma^2_{g,2}$.

These assumptions are common in the bilevel optimization literature (Ghadimi & Wang, 2018; Chen et al., 2021a; Ji et al., 2021). Assumption A requires that the inner and outer functions are well-behaved. Specifically, strong-convexity of the inner objective is a recurring assumption in bilevel optimization theory implying a unique solution to the inner minimization in (1).

2.2. Proposed Algorithm: \textsc{FedNest}

In this section, we develop \textsc{FedNest}, which is formally presented in Algorithm 1. The algorithm operates in two nested loops. The outer loop operates in rounds $k \in \{1, \ldots, K\}$. Within each round, an inner loop operating for $T$ iterations is executed. Given estimates $x^k$ and $y^k$, each iteration $t \in \{1, \ldots, T\}$ of the inner loop produces a new global model $y^{k,t+1}$ of the inner optimization variable $y^*(x^k)$ as the output of an optimizer \textsc{FedINN}. The final estimate $y^{k+1} = y^{k,T}$ of the inner variable is then used by an optimizer \textsc{FedOUT} to update the outer global model $x^{k+1}$.

The subroutines \textsc{FedINN} and \textsc{FedOUT} are gradient-based optimizers. Each subroutine involves a certain number of
local training steps indexed by $\nu \in \{0, \ldots, \tau_i - 1\}$ that are performed at the $i$th client. The local steps of FedINN iterate over local models $y_{\nu}$ of the inner variable. Accordingly, FedOUT iterates over local models $x_{i,\nu}$ of the global variable. A critical component of FedOUT is a communication-efficient federated hypergradient estimation routine, which we call FedIHGP. The implementation of FedINN, FedOUT and FedIHGP is critical to circumvent the algorithmic challenges of federated bilevel optimization. In the remaining of this section, we detail the challenges and motivate our proposed implementations. Later, in Section 3, we provide a formal convergence analysis of FedNEST.

### 2.3. Key Challenge: Federated Hypergradient Estimation

FedOUT is a gradient-based optimizer for the outer minimization in (1); thus each iteration involves computing $\nabla f(x) = (1/m) \sum_{i=1}^m \nabla f_i(x, y^*(x))$. Unlike single-level FL, the fact that the outer objective $f$ depends explicitly on the inner minimizer $y^*(x)$ introduces a new challenge. A good starting point to understand the challenge is the following evaluation of $\nabla f(x)$ in terms of partial derivatives. The result is well-known from properties of implicit functions.

**Lemma 2.1.** Under Assumption A, for all $i \in [m]$:

$$\nabla f_i(x, y^*(x)) = \nabla^2 f_i(x, y^*(x)) + \nabla^1 f_i(x, y^*(x)),$$

where the direct and indirect gradient components are:

$$\nabla^2 f_i(x, y^*(x)) := \nabla_x f_i(x, y^*(x)), \quad \nabla^1 f_i(x, y^*(x)) := -\nabla^2_{xy} g(x, y^*(x)) \cdot \left[\nabla^2_{yy} g(x, y^*(x))\right]^{-1} \nabla_y f_i(x, y^*(x)).$$

We now use the above formula to describe the two core challenges of bilevel FL optimization.

First, evaluation of any of the terms in (4) requires access to the minimizer $y^*(x)$ of the inner problem. On the other hand, one may at best hope for a good approximation to $y^*(x)$ produced by the inner optimization subroutine. Of course, this challenge is inherent in any bilevel optimization setting, but is exacerbated in the FL setting because of client drift. Specifically, when clients optimize their individual (possibly different) local inner objectives, the global estimate of the inner variable produced by SGD-type methods may drift far from (a good approximation to) $y^*(x)$. We explain in Section 2.5 how FedINN solves that issue.

The second challenge comes from the stochastic nature of the problem. Observe that the indirect component in (4b) is nonlinear in the Hessian $\nabla^2_{xy} g(x, y^*(x))$, complicating an unbiased stochastic approximation of $\nabla f_i(x, y^*(x))$. As we expose here, solutions to this complication developed in the non-federated bilevel optimization literature, are not directly applicable in the FL setting. Indeed, existing stochastic bilevel algorithms, e.g. (Ghadimi & Wang, 2018), define $\nabla^0 f(x, y) := \nabla^2 f(x, y) + \nabla^1 f(x, y)$ as a surrogate of $\nabla f(x, y^*(x))$ by replacing $y^*(x)$ in definition (4) with an approximation $y$ and using the following stochastic approximations:

$$\nabla^0 f(x, y) \approx \nabla_x f(x, \hat{y}), \quad \nabla^1 f(x, y) \approx -\nabla^2_{xy} g(x, y^*(x)),$$

$$\frac{N}{N'} \prod_{\ell=1}^{N'} \left( \frac{1}{\ell g, 1} \nabla^2_{yy} g(x, y^*(x)) \right) \nabla_y f(x, \hat{y}).$$

Here, $N'$ is drawn from $\{0, \ldots, N-1\}$ uniformly at random (UAR) and $\{\hat{y}, \xi_1, \ldots, \xi_{N'}\}$ are i.i.d. samples. Ghadimi & Wang (2018); Hong et al. (2020) have shown that using (5), the inverse Hessian estimation bias exponentially decreases with the number of samples $N$.

One might hope to directly leverage the above approach in a local computation fashion by replacing the global outer function $f$ with the individual function $f_i$. However, note from (4b) and (5b) that the proposed stochastic approximation of the indirect gradient involves in a nonlinear way the global Hessian, which is not available at the client).

Communication efficiency is one of the core objectives of FL, making the idea of communicating Hessians between clients and server prohibitive. Is it then possible, in a FL setting, to obtain an accurate stochastic estimate of the indirect gradient while retaining communication efficiency? In Section 2.4, we show how FedOUT and its subroutine FedIHGP, a matrix-vector products-based (thus, communication efficient) federated hypergradient estimator, answer this question affirmatively.

### 2.4. Outer Optimizer: FedOUT

This section presents the outer optimizer FedOUT, formally described in Algorithm 2. As a subroutine of FedNEST (see Line 9, Algorithm 1), at each round $k = 0, \ldots, K-1$, FedOUT takes the most recent global outer model $x^k$ together with the updated (by FedINN) global inner model $y^{k+1}$ and produces an update $x^{k+1}$. To lighten notation, for a round $k$, denote the function’s input as $(x, y^+)$ (instead of $(x^k, y^{k+1})$) and the output as $x^+$ (instead of $x^{k+1}$). For each client $i \in S$, FedOUT uses stochastic approximations of $\nabla^1 f_i(x, y^+)$ and $\nabla^0 f_i(x, y^+)$, which we call $h^0_i(x, y^+)$ and $h^1_i(x, y^+)$, respectively. The specific choice of these approximations (see Line 5) is critical and is discussed in detail later in this section. Before that, we explain

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2We note that the approximation in (5) is not the only construction, and bilevel optimization can accommodate other forms of gradient surrogates (Ji et al., 2021). Yet, all these approximations require access (in a nonlinear fashion) to the global Hessian; thus, in the same challenge in FL setting.
how each client uses these proxies to form local updates of the outer variable. In each round, starting from a common global model \( x_{i,0} = x \), each client \( i \) performs \( \tau_i \) local steps (in parallel):

\[
x_{i,v+1} = x_{i,v} - \alpha_i h_{i,v},
\]

and then the server aggregates local models via \( x^+ = \sum_{i \in S} x_{i,\tau_i} \). Here, \( \alpha_i \in (0, \alpha] \) is the local stepsize,

\[
\begin{align*}
\hat{h}_{i,v} & := h_i(x, y^+) + h^0(x, y^+) - h^0(x_{i,v}, y^+), \\
\hat{h}_{i,v} & := |S|^{-1} \sum_{i \in S} h_{i,v} = \sum_{i \in S} h_{i,v} - h_i(x, y^+).
\end{align*}
\]

The key features of updates (6)–(7) are exploiting past gradients (variance reduction) to account for objective heterogeneity. Indeed, the ideal update in \textsc{FedOut} would perform the update \( x_{i,v+1} = x_{i,v} - \alpha_i (h^0(x_{i,v}, y^+) + h^0(x_{i,v}, y^+)) \) using the global gradient estimates. But this requires each client \( i \) to have access to both direct and indirect gradients of all other clients—which it does not, since clients do not communicate between rounds. To overcome this issue, each client \( i \) uses global gradient estimates, i.e., \( h^0(x, y^+) + h^0(x_{i,v}, y^+) \) from the beginning of each round as a guiding direction in its local update rule. However, since both \( h^0 \) and \( h^1 \) are computed at a previous \( x, y^+ \), client \( i \) makes a correction by subtracting off the stale direct gradient estimate \( h_i^0(x, y^+) \) and adding its own local estimate \( h_i^0(x_{i,v}, y^+) \). Our local update rule in Step 11 of Algorithm 2 is precisely of this form, i.e., \( h_{i,v} \approx h^0(x_{i,v}, y^+) + h^0(x_{i,v}, y^+) \) via (7). Note here that the described local correction of \textsc{FedOut} only applies to the direct gradient component (the indirect component would require global Hessian information). An alternative approach leading to \textsc{FedNEST} is discussed in Section 2.6.

**\textsc{FedOut} applied to special nested problems.** Algorithm 2 naturally allows the use of other optimizers for minimax & compositional optimization. For example, in the minimax problem (2), the bilevel gradient components are \( \nabla_x f_i(x, y^+(x)) = \nabla_x f_i(x, y^+(x)) \) and \( \nabla_y f_i(x, y^+(x)) = 0 \) for all \( i \in S \). Hence, the hypergradient estimate (7) reduces to

\[
h_{i,v} = h^0(x, y^+) - h_i^0(x_{i,v}, y^+) + h_i^0(x_{i,v}, y^+) .
\]

For the compositional problem (3), Hessian becomes the identity matrix, the direct gradient is the zero vector, and \( \nabla_{xy} g_i(x, y) = -(1/m) \sum_{i=1}^{m} \nabla r_i(x)^\top \). Hence, \( h_i = \xi g_i \nabla r_i(x)^\top p_0 \) for all \( i \in S \).

More details on these special cases are provided in Appendices D and E.

**Indirect gradient estimation & \textsc{FedIHGP.** Here, we aim to address one of the key challenges in nested FL: inverse Hessian gradient product. Note from (5b) that the proposed stochastic approximation of the indirect gradient involves in a nonlinear way the global Hessian, which is not available at the client. To get around this, we use a client sampling strategy and recursive reformulation of (5b) so that \( \nabla_i f_i(x, y) \) can be estimated in an efficient federated manner. In particular, given \( N \in \mathbb{N} \), we select \( N' \in \{0, \ldots, N-1\} \) and \( S_0, \ldots, S_{N'} \subseteq S \) \( UAR \). For all \( i \in S \), we then define

\[
\tilde{h}_i(x, y) = -\nabla^2 g_i(x, y; \xi_i)p_{N'},
\]

where \( p_{N'} = |S_0|^{-1} \tilde{H}_y \sum_{i \in S_0} \nabla y f_i(x, y; \xi_i) \) and \( \tilde{H}_y \)
Algorithm 4 $y^+ = \text{FEDINN}(x, y, \beta)$

1: $G_i(\cdot) \leftarrow \nabla_y g_i(x, \cdot) (\text{bilevel}), -\nabla_y f_i(x, \cdot) (\text{minimax})$
2: $y_{0} = y$ and $\beta_i \in (0, \beta]$
3: for $i \in S$ in parallel do
4: $q_i = G_i(y; \zeta_i)$
5: end for
6: $q = |S|^{-1} \sum_{i \in S} q_i$
7: for $i \in S$ in parallel do
8: for $\nu = 0, \ldots, \tau_i - 1$ do
9: $q_{i,\nu} = G_i(y_{i,\nu}; \zeta_{i,\nu}) - G_i(y; \zeta_{i,\nu}) + q$
10: $y_{i,\nu+1} = y_{i,\nu} - \beta_i q_{i,\nu}$
11: end for
12: end for
13: $y^+ = |S|^{-1} \sum_{i \in S} y_{i,\tau_i}$

2.6. Light-\textsc{FEDNest}: Communication Efficiency via Local Hypergradients

Each \textsc{FEDNest} epoch $k$ requires $2T + N + 3$ communication rounds as follows: $2T$ rounds for SVRG of \textsc{FEDINN}, $N$ iterations for inverse Hessian approximation within \textsc{FEDIHG} and 3 additional aggregations. Note that, these are vector communications and we fully avoid Hessian communication. In Appendix A, we also propose simplified variants of \textsc{FEDOUT} and \textsc{FEDIHG}, which are tailored to homogeneous or high-dimensional FL settings. These algorithms can then either use local Jacobian / inverse Hessian or their approximation, and can use either SVRG or SGD.

\textbf{Light-\textsc{FEDNest}}: Specifically, we propose LF\textsc{EDNest} where each client runs IHGP locally. This reduces the number of rounds to $T + 1$, saving $T + N + 2$ rounds (see experiments in Section 4 for performance comparison and Appendix A for further discussion.)

3. Convergence Analysis for \textsc{FEDNest}

In this section, we present convergence results for \textsc{FEDNest}. All proofs are relegated to Appendices C–E.

Theorem 3.1. Suppose Assumptions A and B hold. Further, assume $\alpha_k = \alpha_k/\tau_i$ and $\beta_k = \beta_k/\tau_i$ for all $i \in S$, where

$$\beta_k = \frac{\beta \alpha_k}{T}, \quad \alpha_k = \min \left\{ \alpha_1, \alpha_2, \alpha_3, \frac{\bar{\alpha}}{\sqrt{K}} \right\}$$

for some positive constants $\alpha_1, \alpha_2, \alpha_3, \bar{\alpha}$, and $\beta$ independent of $K$. Then, for any $T \geq 1$, the iterates $\{(x^k, y^k)\}_{k \geq 0}$ generated by \textsc{FEDNest} satisfy

$$\frac{1}{K} \sum_{k=1}^{K} \mathbb{E} \left[ \|\nabla f(x^k)\|^2 \right] = O \left( \frac{\bar{\alpha} \max(\sigma_{g,1}^2, \sigma_{g,2}^2, \sigma_f^2)}{\sqrt{K}} + \frac{1}{\min(\alpha_1, \alpha_2, \alpha_3) K + b^2} \right),$$
where \( b = \kappa_g \ell f_1 \left( \left( \kappa_g - 1 \right) / \kappa_g \right)^N \) and \( N \) is the input parameter to FedIHGP.

**Corollary 3.1 (Bilevel).** Under the same conditions as in Theorem 3.1, if \( N = O(\kappa_g \log K) \) and \( T = O(\kappa_g^3) \), then

\[
\frac{1}{K} \sum_{k=1}^{K} \mathbb{E} \left[ \left\| \nabla f(x^k) \right\|^2 \right] = O \left( \frac{\kappa_g^2}{K} + \frac{\kappa_f^2}{\sqrt{K}} \right).
\]

For \( \epsilon \)-accurate stationary point, we need \( K = O(\kappa_g^3 \epsilon^{-2}) \).

Above, we choose \( N \sim O(\kappa_g \log K) \) to guarantee \( b^2 \lesssim 1/\sqrt{K} \). In contrast, we use \( T \gtrsim \kappa_g^2 \) inner SVRG epochs. From Section 2.6, this would imply the communication cost is dominated by SVRG epochs \( N \) and \( O(\kappa_g^3) \) rounds.

From Corollary 3.1, we remark that FedNEST matches the guarantees of centralized alternating SGD methods, such as ALSET (Chen et al., 2021a) and BSA (Ghadimi & Wang, 2018), despite federated setting, i.e. communication challenge, heterogeneity in the client objectives, and device heterogeneity.

### 3.1. Minimax Federated Learning

We focus on special features of federated minimax problems and customize the general results to yield improved convergence results for this special case. Recall from (2) that \( g_i(x, y) = -f_i(x, y) \) which implies that \( b = 0 \) and following Assumption A, \( f_i(x, y) \) is \( \mu_f \)-strongly concave in \( y \) for all \( x \).

**Corollary 3.2 (Minimax).** Denote \( \kappa_f = \ell f_1 / \mu_f \). Assume same conditions as in Theorem 3.1 and \( T = O(\kappa_f) \). Then,

\[
\frac{1}{K} \sum_{k=1}^{K} \mathbb{E} \left[ \left\| \nabla f(x^k) \right\|^2 \right] = O \left( \frac{\kappa_f^2}{K} + \frac{\kappa_f^2}{\sqrt{K}} \right).
\]

Corollary 3.2 implies that for the minimax problem, the convergence rate of FedNEST to the stationary point of \( f \) is \( O(1/\sqrt{K}) \). Again, we note this matches the convergence rate of non-FL algorithms (see also Table 1) such as SGDA (Lin et al., 2020) and SMD (Rafique et al., 2021).

### 3.2. Compositional Federated Learning

Observe that in the compositional problem (3), the outer function is \( f_i(x, y; \xi) = f_i(x; \xi) \) and the inner function is \( g_i(x, y; \xi) = 1/2 \left\| y - r_i(x; \xi) \right\|^2 \), for all \( i \in S \). Hence, \( b = 0 \) and \( \kappa_g = 1 \).

**Corollary 3.3 (Compositional).** Under the same conditions as in Theorem 3.1, if we select \( T = 1 \) in (12). Then,

\[
\frac{1}{K} \sum_{k=1}^{K} \mathbb{E} \left[ \left\| \nabla f(x^k) \right\|^2 \right] = O \left( \frac{1}{\sqrt{K}} \right).
\]

Corollary 3.3 implies that for the compositional problem (3), the convergence rate of FedNEST to the stationary point of \( f \) is \( O(1/\sqrt{K}) \). This matches the convergence rate of non-federated stochastic algorithms such as SCGD (Wang et al., 2017) and NASA (Ghadimi et al., 2020) (Table 1).

### 3.3. Single-Level Federated Learning

Building upon the general results for stochastic nonconvex nested problems, we establish new convergence guarantees for single-level stochastic non-convex federated SVRG which is integrated within our FedOUT. Note that in the single-level setting, the optimization problem (1) reduces to

\[
\min_{x \in \mathbb{R}^d} f(x) = \frac{1}{m} \sum_{i=1}^{m} f_i(x)
\]

with \( f_i(x) := \mathbb{E}_{\xi \sim C_i} [f_i(x; \xi)] \), where \( \xi \sim C_i \) is sampling distribution for the \( i^{th} \) client.

We make the following assumptions on (13) that are counterparts of Assumptions A and B.

**Assumption C (Lipschitz continuity).** For all \( i \in [m] \), \( \nabla f_i(x) \) is \( L_f \)-Lipschitz continuous.

**Assumption D (Stochastic samples).** For all \( i \in [m] \), \( \nabla f_i(x; \xi) \) is an unbiased estimator of \( \nabla f_i(x) \) and its variance is bounded, i.e., \( \mathbb{E}_\xi [\| \nabla f_i(x; \xi) - \nabla f_i(x) \|^2] \leq \sigma_i^2 \).

**Theorem 3.2 (Single-Level).** Suppose Assumptions C and D hold. Further, assume \( \alpha_i^2 = \alpha_k / \tau_i \) for all \( i \in S \), where

\[
\alpha_k = \min \left\{ \bar{\alpha}_1, \frac{\bar{\alpha}}{} \right\}
\]

for some \( \bar{\alpha}_1, \bar{\alpha} > 0 \). Then,

\[
\frac{1}{K} \sum_{k=1}^{K} \mathbb{E} \left[ \left\| \nabla f(x^k) \right\|^2 \right] = O \left( \frac{\Delta_f}{\bar{\alpha}_1 K} + \frac{\Delta_f}{\bar{\alpha} \sqrt{K}} \right)
\]

where \( \Delta_f := f(x^0) - \mathbb{E}[f(x^K)] \).

Theorem 3.2 extends recent results by (Mitra et al., 2021) from the stochastic strongly convex to the stochastic nonconvex setting. The above rate is also consistent with existing single-level non-FL guarantees (Ghadimi & Lan, 2013).

### 4. Numerical Experiments

In this section, we numerically investigate the impact of several attributes of our algorithms on a hyper-representation problem (Franceschi et al., 2018), a hyper-parameter optimization problem for loss function tuning (Li et al., 2021), and a federated minimax optimization problem.

#### 4.1. Hyper-Representation Learning

Modern approaches in meta learning such as MAML (Finn et al., 2017) and reptile (Nichol & Schulman, 2018) learn...
We use bilevel optimization to tune a loss function for learning an imbalanced MNIST dataset. We aim to maximize the class-balanced validation accuracy (which helps mitigate imbalanced MNIST dataset. We aim to maximize
improves test performance by enabling faster convergence. The inner problem optimizes a header for downstream classification considerations in Section 2.5). To further clarify the algorithm for heterogeneous data (as predicted by our theoretical analysis in Appendix A), FedNest saves on communication rounds compared to FedNest and performs well on homogeneous clients. However, for heterogeneous clients, the isolation of local Hessian in LFedNest (see Algorithm 5 in Appendix A) degrades the test performance. Next, Figure 2b demonstrates the importance of SVRG in FedINN to achieve near non-federated performance.

4.2. Loss Function Tuning on Imbalanced Dataset

We use bilevel optimization to tune a loss function for learning an imbalanced MNIST dataset. We aim to maximize the class-balanced validation accuracy (which helps mitigate imbalanced MNIST dataset. We aim to maximize the class-balanced validation accuracy (which helps mitigate imbalanced MNIST dataset. We aim to maximize
We conduct experiments on the minimax problem (2) with implementation that uses SGD-type updates. The figure confirms our discussion in Section 2.5: SVRG offers significant performance gains that are pronounced by client heterogeneity.

4.3. Federated Minimax Problem

We conduct experiments on the minimax problem (2) with $f_i(x, y) := -\frac{1}{2}\|y\|^2 - b_i^T y + y^T A_i x + \frac{\lambda}{2}\|x\|^2$, to compare standard FEDAVG saddle-point (FEDAVG-S) method updating $(x, y)$ simultaneously (Hou et al., 2021) and our alternative approaches (LFEDNest and FEDNest). This is a saddle-point formulation of $\min_{x \in \mathbb{R}^n} \max_{y \in \mathbb{R}^m} \frac{1}{m} \sum_{i=1}^{m} A_i x - b_i^2$. We set $\lambda = 10$, $b_i = b_i^* - \frac{1}{m} \sum_{i=1}^{m} b_i^*$ and $A_i = I$, where $b_i^* \sim \mathcal{N}(0, s^2 I_d)$, and $t_i$ is drawn UAR over $(0, 0.1)$. Figure 4 shows that LFEDNest and FEDNest outperform FEDAVG-S thanks to their alternating nature. FEDNest significantly improves the convergence of LFEDNest due to controlling client-drift. To our knowledge, FEDNest is the only alternating federated SVRG for minimax problems.

5. Related Work

Federated learning. FEDAVG was first introduced by McMahan et al. (2017), who showed it can dramatically reduce communication costs. For identical clients, FEDAVG coincides with local SGD (Zinkevich et al., 2010) which has been analyzed by many works (Stich, 2019; Yu et al., 2019; Wang & Joshi, 2018). Recently, many variants of FEDAVG have been proposed to tackle issues such as convergence and client drift. Examples include FEDPROX (Li et al., 2020b), SCAFFOLD (Karimireddy et al., 2020), FEDSPLIT (Pathak & Wainwright, 2020), FEDNOVA (Wang et al., 2020), and, the most closely relevant to us, FEDLIN (Mitra et al., 2021). A few recent studies are also devoted to the extension of FEDAVG to the minimax optimization (Rasouli et al., 2020; Deng et al., 2020) and compositional optimization (Huang et al., 2021). In contrast to these methods, FEDNest makes alternating SVRG updates between the global variables $x$ and $y$, and yields sample complexity bounds and batch size choices that are on par with the non-FL guarantees (Table 1). Evaluations in the Appendix H.1 reveal that both alternating updates and SVRG provides a performance boost over these prior approaches.

Bilevel optimization. This class of problems was first introduced by (Bracken & McGill, 1973), and since then, different types of approaches have been proposed. See (Sinha et al., 2017; Liu et al., 2021) for surveys. Earlier works in (Aiyoshi & Shimizu, 1984; Lv et al., 2007) reduced the bilevel problem to a single-level optimization problem. However, the reduced problem is still difficult to solve due to for example a large number of constraints. Recently, more efficient gradient-based algorithms have been proposed by estimating the hypergradient of $\nabla f(x)$ through iterative updates (Maclaurin et al., 2015; Franceschi et al., 2017; Donmez, 2012; Pedregosa, 2016). The asymptotic and non-asymptotic analysis of bilevel optimization has been provided in (Franceschi et al., 2018; Shaban et al., 2019; Liu et al., 2020) and (Ghadimi & Wang, 2018; Hong et al., 2020), respectively. There is also a line of work focusing on minimax optimization (Nemirovski, 2004; Daskalakis & Panageas, 2018) and compositional optimization (Wang et al., 2017). Closely related to our work are (Lin et al., 2020; Rafique et al., 2021; Chen et al., 2021a) and (Ghadimi et al., 2020; Chen et al., 2021a) which provide non-asymptotic analysis of SGD-type methods for minimax and compositional problems with outer nonconvex objective, respectively.

A more in-depth discussion of related work is given in Appendix B. We summarize the complexities of different methods for FL/non-FL bilevel optimization in Table 1.

6. Conclusions

We presented a new class of federated algorithms for solving general nested stochastic optimization spanning bilevel and minimax problems. FEDNest runs a variant of federated SVRG on inner & outer variables in an alternating fashion. We established provable convergence rates for FEDNest under arbitrary client heterogeneity and introduced variations for min-max and compositional problems and for improved communication efficiency (LFEDNest). We showed that, to achieve an $\epsilon$-stationary point of the nested problem, FEDNest requires $O(\epsilon^{-2})$ samples in total, which matches the complexity of the non-federated nested algorithms in the literature.

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APPENDIX

**FedNest: Federated Bilevel, Minimax, and Compositional Optimization**

The appendix is organized as follows: Section A introduces the LFEdNest algorithm. Section B discusses the related work. We provide all details for the proof of the main theorems in Sections C, D, E, and F for federated bilevel, minimax, compositional, and single-level optimization, respectively. In Section G, we state a few auxiliary technical lemmas. Finally, in Section H, we provide the detailed parameters of our numerical experiments (Section 4) and then introduce further experiments.

### A. LFEdNest

Implementing FedINN and FedOUT naively by using the global direct and indirect gradients and sending the local information to the server that would then calculate the global gradients leads to a communication and space complexity of which can be prohibitive for large-sized $d_1$ and $d_2$. One can consider possible local variants of FedINN and FedOUT tailored to such scenarios. Each of the possible algorithms (See Table 2) can then either use the global gradient or only the local gradient, either use a SVRG or SGD.

**Algorithm 5** $x^+ = \text{LFEdOUT} (x, y, \alpha)$ for stochastic bilevel, minimax, and compositional problems

1: $x_{i,0} = x$ and $\alpha_i \in (0, \alpha]$ for each $i \in \mathcal{S}$.
2: Choose $N \in \{1, 2, \ldots\}$ (the number of terms of Neumann series).
3: for $i \in \mathcal{S}$ in parallel do
4:     for $\nu = 0, \ldots, \tau_i - 1$ do
5:         Select $N' \in \{0, \ldots, N - 1\}$ UAR.
6:         $h_{i,\nu} = \nabla_x f_i(x_{i,\nu}, y; \xi_{i,\nu}) - \frac{N}{g_i} \nabla_x g_i(x_{i,\nu}, y; \xi_{i,\nu}) \prod_{n=1}^{N'} \left( I - \frac{1}{g_i} \nabla_x g_i(x_{i,\nu}, y; \xi_{i,n}) \right) \nabla_x f_i(y_{i,\nu}, x_{i,\nu})$
7:         $h_{i,\nu} = \nabla_x f_i(x_{i,\nu}, y; \xi_{i,\nu})$
8:         $h_{i,\nu} = \nabla r_i(x_{i,\nu}; \xi_{i,\nu})^\top \nabla f_i(y_{i,\nu}; \xi_{i,\nu})$
9:         $x_{i,\nu+1} = x_{i,\nu} - \alpha_i h_{i,\nu}$
10:    end for
11: end for
12: $x^+ = |\mathcal{S}|^{-1} \sum_{i \in \mathcal{S}} x_{i,\tau_i}$

**Algorithm 6** $y^+ = \text{LFEdINN} (x, y, \beta)$ for stochastic bilevel, minimax, and compositional problems

1: $y_{i,0} = y$ and $\beta_i \in (0, \beta]$ for each $i \in \mathcal{S}$.
2: for $i \in \mathcal{S}$ in parallel do
3:     for $\nu = 0, \ldots, \tau_i - 1$ do
4:         $q_{i,\nu} = \nabla_y g_i(x, y_{i,\nu}; \xi_{i,\nu})$ $q_{i,\nu} = -\nabla_x f_i(x, y_{i,\nu}; \xi_{i,\nu})$ $q_{i,\nu} = y_{i,\nu} - r_i(x; \xi_{i,\nu})$
5:         $y_{i,\nu+1} = y_{i,\nu} - \beta_i q_{i,\nu}$
6:     end for
7: end for
8: $y^+ = |\mathcal{S}|^{-1} \sum_{i \in \mathcal{S}} y_{i,\tau_i}$
Table 2: Definition of studied algorithms by using inner/outer optimization algorithms and server updates and resulting properties of these algorithms. $T$ and $N$ denote the number of inner iterations and terms of Neumann series, respectively.

**B. Related Work**

We provide an overview of the current literature on non-federated nested (bilevel, minimax, and compositional) optimization and federated learning.

**B.1. Bilevel Optimization**

A broad collection of algorithms have been proposed to solve bilevel nonlinear programming problems. Aiyoshi & Shimizu (1984); Edmunds & Bard (1991); Al-Khayyal et al. (1992); Hansen et al. (1992); Shi et al. (2005); Lv et al. (2007); Moore (2010) reduce the bilevel problem to a single-level optimization problem using for example the Karush-Kuhn-Tucker (KKT) conditions or penalty function methods. A similar idea was also explored in Khodak et al. (2021) where the authors provide a reformulation of the hyperparameter optimization (bilevel objective) into a single-level objective and develop a federated online method to solve it. However, the reduced single-level problem is usually difficult to solve (Sinha et al., 2017).

In comparison, alternating gradient-based approaches designed for the bilevel problems are more attractive due to their simplicity and effectiveness. This type of approaches estimate the hypergradient $\nabla f(x)$ for iterative updates, and are generally divided to approximate implicit differentiation (AID) and iterative differentiation (ITD) categories. ITD-based approaches (Maclaurin et al., 2015; Franceschi et al., 2017; Finn et al., 2017; Grazzi et al., 2020) estimate the hypergradient $\nabla f(x)$ in either a reverse (automatic differentiation) or forward manner. AID-based approaches (Pedregosa, 2016; Grazzi et al., 2020; Ghadimi & Wang, 2018) estimate the hypergradient via implicit differentiation which involves solving a linear system. Our algorithms follow the latter approach.

Theoretically, bilevel optimization has been studied via both asymptotic and non-asymptotic analysis (Franceschi et al., 2018; Liu et al., 2020; Li et al., 2020a; Shaban et al., 2019; Ghadimi & Wang, 2018; Ji et al., 2021; Hong et al., 2020). In particular, (Franceschi et al., 2018) provided the asymptotic convergence of a backpropagation-based approach as one of ITD-based algorithms by assuming the inner problem is strongly convex. (Shaban et al., 2019) gave a similar analysis for a truncated backpropagation approach. Non-asymptotic complexity analysis for bilevel optimization has also been explored. Ghadimi & Wang (2018) provided a finite-time convergence analysis for an AID-based algorithm under three different loss geometries, where $f(\cdot)$ is either strongly convex, convex or nonconvex, and $g(x, \cdot)$ is strongly convex. (Ji et al., 2021) provided an improved non-asymptotic analysis for AID- and ITD-based algorithms under the nonconvex-strongly-convex geometry. (Ji & Liang, 2021) provided the first-known lower bounds on complexity as well as tighter upper bounds. When the objective functions can be expressed in an expected or finite-time form, (Ghadimi & Wang, 2018; Ji et al., 2021; Hong et al., 2020) developed stochastic bilevel algorithms and provided the non-asymptotic analysis. (Chen et al., 2021a) provided a tighter analysis of SGD for stochastic bilevel problems. (Chen et al., 2021b; Guo et al., 2021; Khanduri et al., 2021; Ji et al., 2020a; Huang & Huang, 2021; Dagréou et al., 2022) studied accelerated SGD, SAGA, momentum, and adaptive-type bilevel optimization methods. More results can be found in the recent review paper (Liu et al., 2021) and references therein.
B.1.1. MINIMAX OPTIMIZATION

Minimax optimization has a long history dating back to (Brown, 1951). Earlier works focused on the deterministic convex-concave regime (Nemirovski, 2004; Nedić & Ozdaglar, 2009). Recently, there has emerged a surge of studies of stochastic minimax problems. The alternating version of the gradient descent ascent (SGDA) has been studied by incorporating the idea of optimism (Daskalakis & Panageas, 2018; Gidel et al., 2018; Mokhtari et al., 2020; Yoon & Ryu, 2021). (Rafique et al., 2021; Thekumparampil et al., 2019; Nouiehed et al., 2019; Lin et al., 2020) studied SGDA in the nonconvex-strongly concave setting. Specifically, the $O(\epsilon^{-2})$ sample complexity has been established in (Lin et al., 2020) under an increasing batch size $O(\epsilon^{-1})$. Chen et al. (2021a) provided the $O(\epsilon^{-2})$ sample complexity under an $O(1)$ constant batch size. In the same setting, accelerated GDA algorithms have been developed in (Luo et al., 2020; Yan et al., 2020; Tran Dinh et al., 2020). Going beyond the one-side concave settings, algorithms and their convergence analysis have been studied for nonconvex-nonconcave minimax problems with certain benign structure; see e.g., (Gidel et al., 2018; Liu et al., 2019; Yang et al., 2020; Diakonikolas et al., 2021; Barazandehe et al., 2021b). A comparison of our results with prior work can be found in Table 1.

B.1.2. COMPOSITIONAL OPTIMIZATION

Stochastic compositional gradient algorithms (Wang et al., 2017; 2016) can be viewed as an alternating SGD for the special compositional problem. However, to ensure convergence, the algorithms in (Wang et al., 2017; 2016) use two sequences of variables being updated in two different time scales, and thus the iteration complexity of (Wang et al., 2017) and (Wang et al., 2016) is worse than $O(\epsilon^{-2})$ of the standard SGD. Our work is closely related to ALSET (Chen et al., 2021a), where an $O(\epsilon^{-2})$ sample complexity has been established in a non-FL setting.

B.2. Federated Learning

FL involves learning a centralized model from distributed client data. Although this centralized model benefits from all client data, it raises several types of issues such as generalization, fairness, communication efficiency, and privacy (Mohri et al., 2019; Stich, 2019; Yu et al., 2019; Wang & Joshi, 2018; Stich & Karimireddy, 2019; Basu et al., 2019; Nazari et al., 2019; Barazandehe et al., 2021a). FEDAVG (McMahan et al., 2017) can tackle some of these issues such as high communication costs. Many variants of FEDAVG have been proposed to tackle other emerging issues such as convergence and client drift. Examples include adding a regularization term in the client objectives towards the broadcast model (Li et al., 2020b), proximal splitting (Pathak & Wainwright, 2020; Mitra et al., 2021), variance reduction (Karimireddy et al., 2020; Mitra et al., 2021) and adaptive updates (Reddi et al., 2020). When clients are homogeneous, FEDAVG is closely related to local SGD (Zinkevich et al., 2010), which has been analyzed by many works (Stich, 2019; Yu et al., 2019; Wang & Joshi, 2018; Stich & Karimireddy, 2019; Basu et al., 2019).

In order to analyze FEDAVG in heterogeneous settings, (Li et al., 2020b; Wang et al., 2019; Khaled et al., 2019; Li et al., 2019) derive convergence rates depending on the amount of heterogeneity. They showed that the convergence rate of FEDAVG gets worse with client heterogeneity. By using control variates to reduce client drift, the SCAFFOLD method (Karimireddy et al., 2020) achieves convergence rates that are independent of the amount of heterogeneity. Relatedly, FEDNOVA (Wang et al., 2020) and FEDLIN (Mitra et al., 2021) provided the convergence of their methods despite arbitrary local objective and systems heterogeneity. In particular, (Mitra et al., 2021) showed that FEDLIN guarantees linear convergence to the global minimum of deterministic objective, despite arbitrary objective and systems heterogeneity. As explained in the main body, our algorithms critically leverage these ideas after identifying the additional challenges that client drift brings to federated bilevel settings.

B.2.1. FEDERATED MINIMAX LEARNING

A few recent studies are devoted to federated minimax optimization (Rasouli et al., 2020; Reisizadeh et al., 2020; Deng et al., 2020; Hou et al., 2021). In particular, (Reisizadeh et al., 2020) consider minimax problem with inner problem satisfying PL condition and the outer one being either nonconvex or satisfying PL. However, the proposed algorithm only communicates $\pi$ to the server. Xie et al. (2021) consider a general class of nonconvex-PL minimax problems in the cross-device federated learning setting. Their algorithm performs multiple local update steps on a subset of active clients in each round and leverages global gradient estimates to correct the bias in local update directions. Deng & Mahdavi (2021) studied federated optimization for a family of smooth nonconvex minimax functions. Shen et al. (2021) proposed a distributed minimax optimizer called FEDMM, designed specifically for the federated adversary domain adaptation problem.
Hou et al. (2021) proposed a SCAFFOLD saddle point algorithm (SCAFFOLD-S) for solving strongly convex-concave minimax problems in the federated setting. To the best of our knowledge, all the aforementioned developments require a bound on the heterogeneity of the local functions, and do not account for the effects of systems heterogeneity which is also a key challenge in FL. In addition, our work proposes the first alternating federated SVRG-type algorithm for minimax problems with iteration complexity that matches to the non-federated setting (see, Table 1).

C. Proof for Federated Bilevel Optimization

Throughout the proof, we will use $\mathcal{F}_{i,t}^{k}$ to denote the filtration that captures all the randomness up to the $\nu$-th local step of client $i$ in inner round $t$ and outer round $k$. With a slight abuse of notation, $\mathcal{F}_{i,-1}^{k}$ is to be interpreted as $\mathcal{F}_{i,t}^{k}, \forall i \in \mathcal{S}$. For simplicity, we remove subscripts $k$ and $t$ from the definition of stepsizes and model parameters. For example, $x$ and $x^+$ denote $x^k$ and $x^{k+1}$, respectively. We further set

$$h_i(x_{i,\nu}, y^+):= \mathbb{E}[h_i(x_{i,\nu}, y^+)|\mathcal{F}_{i,\nu-1}].$$

Proof of Lemma 2.1

Proof. Given $x \in \mathbb{R}^d$, the optimality condition of the inner problem in (1) is $\nabla g(x, y) = 0$. Now, since $\nabla_x (\nabla_y g(x, y)) = 0$, we obtain

$$0 = \sum_{j=1}^{m} \left( \nabla^2_{xy} g_j (x, y^*(x)) + \nabla y^*(x) \nabla^2_{y} g_j (x, y^*(x)) \right),$$

which implies

$$\nabla y^*(x) = - \left( \sum_{j=1}^{m} \nabla^2_{xy} g_j (x, y^*(x)) \right)^{-1} \left( \sum_{i=1}^{m} \nabla^2_{y} g_i (x, y^*(x)) \right).$$

The results follows from a simple application of the chain rule to $f$ as follows:

$$\nabla f(x, y^*(x)) = \nabla_x f(x, y^*(x)) + \nabla y^*(x) \nabla_y f(x, y^*(x)).$$

Proof of Lemma 2.2

Proof. By independency of $N'$, $\zeta_{i,n}$, and $\mathcal{S}_n$, and under Assumption B, we have

$$\mathbb{E}_{\mathcal{W}} \left[ \mathcal{H}_y \right] = \mathbb{E}_{\mathcal{W}} \left[ \frac{N}{\ell_{g,1}} \prod_{n=1}^{N'} \left( I - \frac{1}{\ell_{g,1}|\mathcal{S}_n|} \sum_{i=1}^{\left| \mathcal{S}_n \right|} \nabla^2_{y} g_i(x, y; \zeta_{i,n}) \right) \right]$$

$$= \mathbb{E}_{N'} \left[ \mathbb{E}_{\mathcal{S}_n,N'} \left[ \mathbb{E}_{\zeta} \left[ \frac{N}{\ell_{g,1}} \prod_{n=1}^{N'} \left( I - \frac{1}{\ell_{g,1}|\mathcal{S}_n|} \sum_{i=1}^{\left| \mathcal{S}_n \right|} \nabla^2_{y} g_i(x, y; \zeta_{i,n}) \right) \right] \right] \right]$$

$$= \frac{1}{\ell_{g,1}} \sum_{n=0}^{N-1} \left( I - \frac{1}{\ell_{g,1}} \nabla^2_{y} g(x, y) \right)^n,$$

(16)

where the last equality follows from the uniform distribution of $N'$.

Note that since $I \geq \frac{1}{\ell_{g,1}} \nabla^2_{y} g_i \geq \frac{\mu_g}{\ell_{g,1}}$ for all $i \in [m]$ due to Assumption A, we have

$$\mathbb{E}_{\mathcal{W}} \left[ \left\| \mathcal{H}_y \right\| \right] \leq \frac{N}{\ell_{g,1}} \mathbb{E}_{\mathcal{W}} \left[ \prod_{n=1}^{N'} \left( I - \frac{1}{\ell_{g,1}|\mathcal{S}_n|} \sum_{i=1}^{\left| \mathcal{S}_n \right|} \nabla^2_{y} g_i(x, y; \zeta_{i,n}) \right) \right]$$

$$\leq \frac{N}{\ell_{g,1}} \mathbb{E}_{N'} \left[ 1 - \frac{\mu_g}{\ell_{g,1}} \right]^{N'} = \frac{1}{\ell_{g,1} \sum_{n=0}^{N-1} \left[ 1 - \frac{\mu_g}{\ell_{g,1}} \right]^{n}} \leq \frac{1}{\mu_g}.$$

The remainder of the proof is similar to (Ghadimi & Wang, 2018).
The following lemma extends (Ghadimi & Wang, 2018, Lemma 2.2) and (Chen et al., 2021a, Lemma 2) to the finite-sum problem (1). Proofs follow similarly by applying their analysis to the inner and outer functions \( (f_i, g_i) \), \( \forall i \in S \).

**Lemma C.1.** Under Assumptions A and B, for all \( x_1, x_2 \):

\[
\|\nabla f(x_1) - \nabla f(x_2)\| \leq L_f \|x_1 - x_2\|, \\
\|y^*(x_1) - y^*(x_2)\| \leq L_y \|x_1 - x_2\|, \\
\|\nabla y^*(x_1) - \nabla y^*(x_2)\| \leq L_y x \|x_1 - x_2\|,
\]

(17a) (17b) (17c)

Also, for all \( i \in S, \nu \in \{0, \ldots, \tau_i - 1\}, x_1, x_2, \) and \( y \), we have:

\[
\|\nabla f_i(x_1, y) - \nabla f_i(x_1, y^*(x_1))\| \leq M_f \|y^*(x_1) - y\|, \\
\|\nabla f_i(x_2, y) - \nabla f_i(x_1, y)\| \leq M_f \|x_2 - x_1\|, \\
\mathbb{E} \left[ \|\hat{h}_i(x_{i, \nu}, y) - h_i(x_{i, \nu}, y)\|^2 \right] \leq \hat{\sigma}_f^2, \\
\mathbb{E} \left[ \|\hat{h}_i(x_{i, \nu}, y^+)\|^2 \right] \leq \hat{D}_f^2.
\]

(17d) (17e) (17f) (17g)

Here,

\[
L_y := \frac{\ell_{g,1}}{\mu_g} = \mathcal{O}(\kappa_g), \\
L_{yx} := \frac{\ell_{g,2} + \ell_{g,2} L_y}{\mu_g} + \frac{\ell_{g,1}}{\mu_g} \left( \ell_{g,2} + \ell_{g,2} L_y \right) = \mathcal{O}(\kappa_g^3), \\
M_f := \ell_{f,1} + \frac{\ell_{g,1} \ell_{f,1}}{\mu_g} + \frac{\ell_{f,0}}{\mu_g} \left( \ell_{g,2} + \frac{\ell_{g,1} \ell_{g,2}}{\mu_g} \right) = \mathcal{O}(\kappa_g^2), \\
L_f := \ell_{f,1} + \frac{\ell_{g,1} (\ell_{f,1} + M_f)}{\mu_g} + \frac{\ell_{f,0}}{\mu_g} \left( \ell_{g,2} + \frac{\ell_{g,1} \ell_{g,2}}{\mu_g} \right) = \mathcal{O}(\kappa_g^3), \\
\hat{\sigma}_f^2 := \sigma_f^2 + \frac{3}{\mu_g^2} \left( \sigma_f^2 + \ell_{f,0} \right) (\sigma_g^2 + 2 \ell_{g,1}^2) + \sigma_{f,1}^2, \\
\hat{D}_f^2 := \left( \ell_{f,0} + \frac{\ell_{g,1}}{\mu_g} \ell_{f,1} + \ell_{g,1} \ell_{f,1} \frac{1}{\mu_g} \right)^2 + \hat{\sigma}_f^2 = \mathcal{O}(\kappa_g^2),
\]

where the other constants are provided in Assumptions A and B.

**C.1. Descent of Outer Objective**

The following lemma characterizes the descent of the outer objective.

**Lemma C.2** (Descent Lemma). Suppose Assumptions A and B hold. Further, assume \( \tau_i \geq 1 \) and \( \alpha_i = \alpha / \tau_i, \forall i \in S \) for some positive constant \( \alpha \). Then, FEDOUT guarantees:

\[
\mathbb{E} \left[ f(x^+) \right] - \mathbb{E} \left[ f(x) \right] \leq -\frac{\alpha}{2} \mathbb{E} \left[ ||\nabla f(x)||^2 \right] + \frac{\alpha^2 L_f}{2} \hat{\sigma}_f^2 \\
-\frac{\alpha}{2} \left( 1 - \alpha L_f \right) \mathbb{E} \left[ \left( \frac{1}{m \tau_i} \sum_{\nu=0}^{\tau_i-1} \|\hat{h}_i(x_{i, \nu}, y^+)\|^2 \right) \right] \\
+ \frac{3\alpha}{2} \left( b^2 + M_f^2 \mathbb{E} \left[ ||y^* - y^+(x)||^2 \right] + \frac{M_f^2}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \mathbb{E} \left[ ||x_{i, \nu} - x^2 || \right] \right).
\]

(19)

**Proof.** It follows from Algorithm 2 that \( x_{i,0} = x, \forall i \in S \), and

\[
x^+ = x - \frac{1}{m} \sum_{i=1}^{m} \alpha_i \sum_{\nu=0}^{\tau_i-1} h_i(x_{i, \nu}, y^+) .
\]

(20)
Now, using the Lipschitz property of $\nabla f$ in Lemma C.1, we have

$$\mathbb{E}[f(x^+)] - \mathbb{E}[f(x)] \leq \mathbb{E}[\langle x^+ - x, \nabla f(x) \rangle] + \frac{L_f}{2} \mathbb{E}[\|x^+ - x\|^2]$$

$$= -\mathbb{E}\left[\left\langle \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+), \nabla f(x) \right\rangle \right] + \frac{L_f}{2} \mathbb{E}\left[\left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+ ) \right\|^2 \right].$$ (21)

In the following, we bound each term on the right hand side (RHS) of (21). For the first term, we have

$$-\mathbb{E}\left[\left\langle \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+), \nabla f(x) \right\rangle \right] = -\mathbb{E}\left[\left\langle \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} \mathbb{E}[h_i(x_{i,\nu}, y^+), \nabla f(x) | F_{i,\nu-1}] \right\rangle \right]$$

$$= -\mathbb{E}\left[\left\langle \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} \mathbb{E}[h_i(x_{i,\nu}, y^+), \nabla f(x) \| F_{i,\nu-1}] \right\rangle \right]$$

$$= -\frac{\alpha}{2} \mathbb{E}\left[\left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} \mathbb{E}[h_i(x_{i,\nu}, y^+), \nabla f(x) \| F_{i,\nu-1}] \right\|^2 \right] - \frac{\alpha}{2} \mathbb{E}[\|\nabla f(x)\|^2]$$

$$+ \frac{\alpha}{2} \mathbb{E}\left[\left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} \mathbb{E}[h_i(x_{i,\nu}, y^+), \nabla f(x) \| F_{i,\nu-1}] \right\|^2 \right].$$ (22)

where the first equality follows from the law of total expectation; the second equality uses the fact that $\mathbb{E}[h_i(x_{i,\nu}, y^+)] = \mathbb{E}[h_i(x_{i,\nu}, y^+)|F_{i,\nu-1}]$; and the last equality is obtained from our assumption $\alpha_i = \alpha/\tau_i, \forall i \in \mathcal{S}$.

Next, we bound the last term in (22). Note that

$$\left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \mathbb{E}[h_i(x_{i,\nu}, y^+), \nabla f(x) \| F_{i,\nu-1}] \right\|^2 = \left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} (\mathbb{E}[h_i(x_{i,\nu}, y^+), \nabla f_i(x, y^+)])$$

$$+ \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \nabla f_i(x, y^+) - \nabla f(x) \right\|^2$$

$$\leq 3 \left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} (\mathbb{E}[h_i(x_{i,\nu}, y^+), \nabla f_i(x_{i,\nu}, y^+)])$$

$$+ 3 \left\| \nabla f_i(x_{i,\nu}, y^+) - \nabla f_i(x, y^+) \right\|^2 + 3 \left\| \nabla f(x, y^+) - \nabla f(x) \right\|^2,$$

where the inequality uses Lemma G.1.

Hence,

$$\mathbb{E}\left[\left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \mathbb{E}[h_i(x_{i,\nu}, y^+), \nabla f(x) \| F_{i,\nu-1}] \right\|^2 \right]$$

$$\leq 3b^2 + \frac{3mL^2}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \mathbb{E}[\|x_{i,\nu} - x\|^2] + 3mL^2 \mathbb{E}[\|y^+ - y^*(x)\|^2],$$ (23)

where the inequality uses Lemmas 2.2 and C.1.
Substituting (23) into (22) yields

\[- \mathbb{E} \left[ \frac{1}{m} \sum_{i=1}^{m} \alpha_i \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+), \nabla f(x) \right] \leq -\frac{\alpha}{2} \mathbb{E} \left[ \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \tilde{h}_i(x_{i,\nu}, y^+) \right] \leq -\frac{\alpha}{2} \mathbb{E} \left[ \| \nabla f(x) \|^2 \right] \]

\[
+ \frac{3\alpha}{2} \left( b^2 + M_f^2 \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] + \frac{M_f^2}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \mathbb{E} \left[ \| x_{i,\nu} - x \|^2 \right] \right).
\]

(24)

Next, we bound the second term on the RHS of (21). Observe that

\[
\mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \alpha_i \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+) \right\|^2 \right] = \alpha^2 \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \left( h_i(x_{i,\nu}, y^+) - \tilde{h}_i(x_{i,\nu}, y^+) + \tilde{h}_i(x_{i,\nu}, y^+) \right) \right\|^2 \right]
\]

\[
\leq \alpha^2 \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \tilde{h}_i(x_{i,\nu}, y^+) \right\|^2 \right] + \alpha^2 \tilde{\sigma}_f^2,
\]

where the inequality follows from Lemmas G.3 and C.1.

Plugging (25) and (24) into (21) completes the proof.

☐

C.2. Error of \textsc{FedInn}

The following lemma establishes the progress of \textsc{FedInn}. It should be mentioned that the assumption on \( \beta_i, \forall i \in S \) is identical to the one listed in (Mitra et al., 2021, Theorem 4).

\textbf{Lemma C.3 (Error of \textsc{FedInn}).} \ Suppose Assumptions A and B hold. Further, assume

\[
\tau_i \geq 1, \quad \alpha_i = \frac{\alpha}{\tau_i}, \quad \beta_i = \frac{\beta}{\tau_i}, \quad \forall i \in S,
\]

where \( 0 < \beta < \min\left(1/(6\ell_{g,1}), 1\right) \) and \( \alpha \) is some positive constant. Then, \textsc{FedInn} guarantees:

\[
\mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] \leq \left( 1 - \frac{3\beta \mu_g}{2} \right)^T \mathbb{E} \left[ \| y - y^*(x) \|^2 \right] + 25T \beta^2 \sigma_{g,1}^2, \quad \text{and}
\]

(26a)

\[
\mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] \leq a_1(\alpha) \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+) \right\|^2 \right]
\]

\[
+ a_2(\alpha) \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] + a_3(\alpha) \tilde{\sigma}_f^2.
\]

(26b)

Here,

\[
a_1(\alpha) := L_y^2 \alpha^2 + \frac{L_y \alpha}{4M_f}, \quad a_2(\alpha) := 1 + 4M_f L_y \alpha + \frac{\eta L_{yx} \tilde{D}_f^2 \alpha^2}{2}, \quad a_3(\alpha) := \alpha^2 L_y + \frac{L_{yx} \alpha^2}{2\eta},
\]

(27)

for any \( \eta > 0 \).
Proof. Note that
\[
\mathbb{E} \left[ \|y^+ - y^*(x^+)\|^2 \right] = \mathbb{E} \left[ \|y^+ - y^*(x)\|^2 \right] + \mathbb{E} \left[ \|y^*(x^+) - y^*(x)\|^2 \right] + 2\mathbb{E} \left[ \langle y^+ - y^*(x), y^*(x) - y^*(x^+) \rangle \right].
\]

Bounding the first term in (28):
From (Mitra et al., 2021, Theorem 4), for all \( t \in \{0, \ldots, T - 1\} \), we obtain
\[
\mathbb{E}[\|y^{t+1} - y^*(x)\|^2] \leq \left( 1 - \frac{\beta \mu_g}{2} \right) \mathbb{E}[\|y^t - y^*(x)\|^2] + 25 \beta^2 \sigma_g^2.
\]
which together with our setting \( y^+ = y^T \) implies
\[
\mathbb{E}[\|y^+ - y^*(x)\|^2] \leq \left( 1 - \frac{\beta \mu_g}{2} \right)^T \mathbb{E}[\|y - y^*(x)\|^2] + 25 T \beta^2 \sigma_g^2.
\]

Bounding the second term in (28):
By similar steps as in (25), we have
\[
\mathbb{E} \left[ \|y^*(x^+) - y^*(x)\|^2 \right] \leq L_y^2 \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} h_i(x, y^+) \right\|^2 \right] \leq L_y^2 \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+) \right\|^2 \right] + \alpha^2 L_y^2 \bar{\sigma}^2,
\]
where the inequalities are obtained from Lemmas C.1 and G.3.

Bounding the third term in (28):
Observe that
\[
\mathbb{E} \left[ \langle y^+ - y^*(x), y^*(x) - y^*(x^+) \rangle \right] = -\mathbb{E} \left[ \langle y^+ - y^*(x), \nabla y^*(x)(x^+ - x) \rangle \right] - \mathbb{E} \left[ \langle y^+ - y^*(x), y^*(x^+) - y^*(x) - \nabla y^*(x)(x^+ - x) \rangle \right].
\]
For the first term on the R.H.S. of the above equality, we have
\[
-\mathbb{E}[\langle y^+ - y^*(x), \nabla y^*(x)(x^+ - x) \rangle] = -\mathbb{E} \left[ \langle y^+ - y^*(x), \frac{1}{m} \nabla y^*(x) \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+) \rangle \right] \leq \mathbb{E} \left[ \|y^+ - y^*(x)\| \left\| \frac{1}{m} \nabla y^*(x) \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+) \right\| \right] \leq L_y \mathbb{E} \left[ \|y^+ - y^*(x)\| \left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+) \right\| \right] \leq 2\gamma \mathbb{E} \left[ \|y^+ - y^*(x)\|^2 \right] + \frac{L_y^2 \alpha^2}{8\gamma} \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+) \right\|^2 \right],
\]
where the first equality uses the fact that \( h_i(x_{i,\nu}, y^+) = \mathbb{E} [h_i(x_{i,\nu}, y^+)|F_{i,\nu-1}] \); the second inequality follows from Lemma C.1; and the last inequality is obtained from the Young’s inequality such that \( ab \leq 2\gamma a^2 + \frac{b^2}{8\gamma} \).

Further, using Lemma C.1, we have
\[
-\mathbb{E}[\langle y^+ - y^*(x), y^*(x^+) - y^*(x) - \nabla y^*(x)(x^+ - x) \rangle] \leq \mathbb{E} \left[ \|y^+ - y^*(x)\| \|y^*(x^+) - y^*(x) - \nabla y^*(x)(x^+ - x)\| \right] \leq \frac{L_y \alpha}{2} \mathbb{E} \left[ \|y^+ - y^*(x)\| \|x^+ - x\|^2 \right],
\]
where the inequality follows from Lemma C.1.

From Algorithm 2, we have

\[ x_{i,0} = x, \forall i \in S, \quad \text{and} \quad x_+ = x - \frac{1}{m} \sum_{i=1}^{m} \frac{\tau_i - 1}{\nu} \sum_{\nu=0}^{\tau_i - 1} h_i(x_{i,\nu}, y^+). \]

(34)

Note that \( F_0 = F_{i,0} \) for all \( i \in S \). Hence,

\[
\begin{align*}
\mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \| x^+ - x \|^2 \right] \\
\leq \frac{1}{m} \sum_{i=1}^{m} \frac{\alpha^2}{\tau_i} \sum_{\nu=0}^{\tau_i - 1} \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \| h_i(x_{i,\nu}, y^+) \|^2 | F_{i,\tau_i-1} \right] \\
\leq \alpha^2 \tilde{D}_f^2 \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right],
\end{align*}
\]

(35)

where the last inequality uses Lemma C.1.

Note also that for any \( \eta > 0 \), we have \( 1 \leq \frac{\eta}{2} + \frac{1}{2\eta} \). Combining this inequality with (33) and using (35) give

\[
-\mathbb{E}[\langle y^+ - y^*(x), y^*(x) - y^*(x) - \nabla y^*(x)(x^+ - x) \rangle] \\
\leq \frac{L_{yx} \alpha^2}{2} \mathbb{E} \left[ \| y^+ - y^*(x) \| \| x^+ - x \| \right] \\
\leq \frac{\eta L_{yx}}{4} \mathbb{E} \left[ \| y^+ - y^*(x) \| \| x^+ - x \| \right] + \frac{L_{yx} \alpha^2}{4\eta} \mathbb{E} \left[ \| x^+ - x \| \right] \\
\leq \frac{\eta L_{yx} \tilde{D}_f^2 \alpha^2}{4} \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] + \frac{L_{yx} \alpha^2}{4\eta} \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i - 1} h_i(x_{i,\nu}, y^+) \right\|^2 \right] + \frac{L_{yx} \alpha^2}{4\eta} \tilde{\sigma}_f^2,
\]

(36)

where the last inequality uses (35) and Lemma 2.2.

Let \( \gamma = M_f L_y \alpha \). Plugging (36) and (32) into (31), we have

\[
\mathbb{E}[\langle y^+ - y^*(x), y^*(x) - y^*(x) \rangle] \leq \left( 2\gamma + \frac{\eta L_{yx} \tilde{D}_f^2 \alpha^2}{2} \right) \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] \\
+ \left( \frac{L_{yx} \alpha^2}{8\gamma} + \frac{L_{yx} \alpha^2}{4\eta} \right) \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i - 1} h_i(x_{i,\nu}, y^+) \right\|^2 \right] + \frac{L_{yx} \alpha^2}{4\eta} \tilde{\sigma}_f^2
\]

(37)

Substituting (37), (30), and (29) into (28) completes the proof. □

C.3. Drifting Errors of FedOUT

The following lemma provides a bound on the drift of each \( x_{i,\nu} \) from \( x \) for stochastic nonconvex bilevel problems. It should be mentioned that similar drifting bounds for single-level problems are provided under either strong convexity (Mitra et al., 2021) and/or bounded dissimilarity assumptions (Wang et al., 2020; Reddi et al., 2020; Li et al., 2020b).

**Lemma C.4 (Drifting Error of FedOUT).** Suppose Assumptions A and B hold. Further, assume \( \tau_i \geq 1 \) and \( \alpha_i \leq 1/(5M_f \tau_i) \), \( \forall i \in S \). Then, for each \( i \in S \) and \( \forall \nu \in \{0, \ldots, \tau_i - 1\} \), FedOUT guarantees:

\[
\mathbb{E} \left[ \| x_{i,\nu} - x \|^2 \right] \leq 36\tau_i^2 \alpha_i^2 \left( M_f^2 \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] + \mathbb{E} \left[ \| \nabla f(x) \|^2 \right] + b^2 \right) \\
+ 27\tau_i \alpha_i^2 \tilde{\sigma}_f.
\]

(38)
Proof. The result trivially holds for $\tau_i = 1$. Let $\tau_i > 1$ and define

$$v_{i,\nu} := \bar{h}_i(x_{i,\nu}, y^+) - \nabla f_i(x_{i,\nu}, y^+) - h_i(x, y^+)$$
$$+ \nabla f_i(x, y^+) + \bar{h}_i(x, y^+) - \nabla f(x, y^+),$$
$$w_{i,\nu} := h_i(x_{i,\nu}, y^+) - \bar{h}_i(x_{i,\nu}, y^+) + h_i(x, y^+)$$
$$- h_i(x, y^+) + h(x, y^+) - \bar{h}(x, y^+),$$
$$z_{i,\nu} := \nabla f_i(x_{i,\nu}, y^+) - \nabla f_i(x, y^+) + \nabla f(x, y^+) - \nabla f(x) + \nabla f(x).$$

(39)

One will notice that

$$v_{i,\nu} + w_{i,\nu} + z_{i,\nu} = h_i(x_{i,\nu}, y^+) - h_i(x, y^+) + h(x, y^+).$$

Hence, from Algorithm 2, for each $i \in S$, and $\forall \nu \in \{0, \ldots, \tau_i - 1\}$, we have

$$x_{i,\nu+1} - x = x_{i,\nu} - x - \alpha_i(v_{i,\nu} + w_{i,\nu} + z_{i,\nu}),$$

(40)

which implies that

$$\mathbb{E} [\|x_{i,\nu+1} - x\|^2] = \mathbb{E} [\|x_{i,\nu} - x - \alpha_i(v_{i,\nu} + w_{i,\nu} + z_{i,\nu})\|^2] + \alpha_i^2 \mathbb{E} [\|w_{i,\nu}\|^2]$$
$$- 2\mathbb{E} [\langle x_{i,\nu} - x - \alpha_i(v_{i,\nu} + w_{i,\nu} + z_{i,\nu}), \alpha_i w_{i,\nu} \rangle | F_{i,\nu-1}]$$
$$= \mathbb{E} [\|x_{i,\nu} - x - \alpha_i(v_{i,\nu} + w_{i,\nu} + z_{i,\nu})\|^2] + \alpha_i^2 \mathbb{E} [\|w_{i,\nu}\|^2].$$

(41)

Here, the last equality uses Lemma G.3 since $\mathbb{E}[w_{i,\nu}|F_{i,\nu-1}] = 0$, by definition.

From Lemmas G.1, 2.2, and C.1, for $v_{i,\nu}$, $w_{i,\nu}$, and $z_{i,\nu}$ defined in (39), we have

$$\mathbb{E} [\|v_{i,\nu}\|^2] \leq 3\mathbb{E} [\|\nabla f_i(x_{i,\nu}, y^+) - \bar{h}_i(x_{i,\nu}, y^+)\|^2]$$
$$+ \|\bar{h}_i(x, y^+) - \nabla f_i(x, y^+)\|^2 + \|\nabla f(x, y^+) - \bar{h}(x, y^+)\|^2]$$
$$\leq 9\beta^2,$$

(42a)

$$\mathbb{E} [\|w_{i,\nu}\|^2] \leq 3\mathbb{E} [\|h_i(x_{i,\nu}, y^+) - \bar{h}_i(x_{i,\nu}, y^+)\|^2]$$
$$+ \|\bar{h}_i(x, y^+) - h_i(x, y^+)\|^2 + \|h(x, y^+) - \bar{h}(x, y^+)\|^2]$$
$$\leq 9\sigma_f^2,$$

(42b)

and

$$\mathbb{E} [\|z_{i,\nu}\|^2] \leq 3\mathbb{E} [\|\nabla f_i(x_{i,\nu}, y^+) - \nabla f_i(x, y^+)\|^2]$$
$$+ \|\nabla f(x, y^+) - \nabla f(x)\|^2 + \|\nabla f(x)\|^2\|]$$
$$\leq 3 \left( M_f^2 \mathbb{E} [\|x_{i,\nu} - x\|^2] + M_f^2 \mathbb{E} [\|y^+ - y^*(x)\|^2] + \mathbb{E} [\|\nabla f(x)\|^2]\right).$$

(42c)

Now, the first term in the RHS of (41) can be bounded as follows:

$$\mathbb{E} [\|x_{i,\nu} - x - \alpha_i(v_{i,\nu} + z_{i,\nu})\|^2] \leq \left(1 + \frac{1}{2\tau_i - 1}\right) \mathbb{E} [\|x_{i,\nu} - x\|^2] + 2\tau_i \mathbb{E} [\|v_{i,\nu} + z_{i,\nu}\|^2]$$
$$\leq \left(1 + \frac{1}{2\tau_i - 1}\right) \mathbb{E} [\|x_{i,\nu} - x\|^2] + 4\tau_i \alpha_i^2 \left( \mathbb{E} [\|z_{i,\nu}\|^2] + \mathbb{E} [\|v_{i,\nu}\|^2]\right)$$
$$\leq \left(1 + \frac{1}{2\tau_i - 1}\right) \mathbb{E} [\|x_{i,\nu} - x\|^2] + 4\tau_i \alpha_i^2 \left( \mathbb{E} [\|z_{i,\nu}\|^2] + 9\beta^2\right)$$
$$\leq \left(1 + \frac{1}{2\tau_i - 1} + 12\tau_i \alpha_i^2 M_f^2\right) \mathbb{E} [\|x_{i,\nu} - x\|^2]$$
$$+ 12\tau_i \alpha_i^2 \left( M_f^2 \mathbb{E} [\|y^+ - y^*(x)\|^2] + \mathbb{E} [\|\nabla f(x)\|^2] + 3\beta^2\right).$$

(43)
Here, the first inequality follows from Lemma G.2; the second inequality uses Lemma G.1; and the third and last inequalities follow from (42a) and (42c).

Substituting (43) into (41) gives
\[
\mathbb{E} \left[ \| x_{i,\nu+1} - x \|^2 \right] \leq \left( 1 + \frac{1}{2\tau_i} + 12\tau_i\alpha_i^2 M_f^2 \right) \mathbb{E} \left[ \| x_{i,\nu} - x \|^2 \right] \\
+ 12\tau_i\alpha_i^2 \left( M_f^2 \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] + \mathbb{E} \left[ \| \nabla f(x) \|^2 \right] + 3\delta^2 \right) + 9\alpha_i^2 \sigma_f^2
\]
\[
\leq \left( 1 + \frac{1}{\tau_i} \right) \mathbb{E} \left[ \| x_{i,\nu} - x \|^2 \right]
\]
\[
+ 12\tau_i\alpha_i^2 \left( M_f^2 \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] + \mathbb{E} \left[ \| \nabla f(x) \|^2 \right] + 3\delta^2 \right) + 9\alpha_i^2 \sigma_f^2.
\] (44)

Here, the first inequality uses (42b) and the last inequality follows by noting \( \alpha_i \leq 1/(5M_f \tau_i) \).

For all \( \tau_i > 1 \), we have
\[
\sum_{j=0}^{\nu-1} \left( 1 + \frac{1}{\tau_i} \right)^j \leq \tau_i \left( 1 + \frac{1}{\tau_i} \right)^\nu \leq \exp (1) \tau_i < 3\tau_i
\] (45)

Now, iterating equation (44) and using \( x_{i,0} = x, \forall i \in S \), we obtain
\[
\mathbb{E} \left[ \| x_{i,\nu} - x \|^2 \right] \leq 12\tau_i\alpha_i^2 \left( M_f^2 \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] + \mathbb{E} \left[ \| \nabla f(x) \|^2 \right] + 3\delta^2 \right) + 9\alpha_i^2 \sigma_f^2 \sum_{j=0}^{\nu-1} \left( 1 + \frac{1}{\tau_i} \right)^j
\]
\[
\leq 3\tau_i \left( 12\tau_i\alpha_i^2 \left( M_f^2 \mathbb{E} \left[ \| y^+ - y^*(x) \|^2 \right] + \mathbb{E} \left[ \| \nabla f(x) \|^2 \right] + 3\delta^2 \right) + 9\alpha_i^2 \sigma_f^2 \right),
\]
where the second inequality uses (45). This completes the proof.

\[\square\]

**Remark C.1.** Lemma C.4 shows that the bound on the client-drift scales linearly with \( \tau_i \) and the inner error \( \| y^+ - y^*(x) \|^2 \) in general nested FL. We aim to control such a drift by selecting \( \alpha_i = O(1/\tau_i) \) for all \( i \in S \) and using the inner error bound provided in Lemma C.3.

Next, we provide the proof of our main result which can be adapted to general nested problems (bilevel, min-max, compositional).

### C.4. Proof of Theorem 3.1

**Proof.** We define the following Lyapunov function
\[
\mathcal{W}^k := f(x^k) + \frac{M_f}{L_y} \| y^k - y^*(x^k) \|^2.
\] (46)

Motivated by (Chen et al., 2021a), we bound the difference between two Lyapunov functions. That is,
\[
\mathcal{W}^{k+1} - \mathcal{W}^k = f(x^{k+1}) - f(x^k) + \frac{M_f}{L_y} (\| y^{k+1} - y^*(x^{k+1}) \|^2 - \| y^k - y^*(x^k) \|^2).
\] (47)

The first two terms on the RHS of (47) quantifies the descent of outer objective \( f \) and the remaining terms measure the descent of the inner errors.

From our assumption, we have \( \alpha_i^k = \alpha_i / \tau_i, \beta_i^k = \beta_i / \tau_i, \forall i \in S \). Substituting these stepsizes into the bounds provided in
where \( a \) and \( b \) are defined in (27).

The above choice of \( W \) guarantees the descent of \( \mathbb{W} \), the following constraints need to be satisfied

\[
\mathbb{W}^{k+1} - \mathbb{W}^k \leq \left( \frac{L_f \alpha_k^2}{2} + \frac{M_f}{L_y} a_3(\alpha_k) \right) \bar{\sigma}_f^2 + \frac{3 \alpha_k b^2}{2},
\]

and

\[
\frac{\alpha_k}{2} \mathbb{E} \left[ \| \nabla f(x^k) \|^2 \right] + \frac{3 M_f^2 \alpha_k^2}{2m} \sum_{i=1}^m \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \mathbb{E} \left[ \| x^k_{i,\nu} - x^k \|^2 \right] 
- \left( \frac{\alpha_k}{2} - \frac{L_f \alpha_k^2}{2} - \frac{M_f}{L_y} a_1(\alpha_k) \right) \mathbb{E} \left[ \| x^k_{i,\nu} - y^k \|^2 \right] 
+ \frac{M_f}{L_y} \left( \frac{3 M_f L_y \alpha_k}{2} + a_2(\alpha_k) \right) \mathbb{E} \left[ \| y^{k+1} - y^* \|^2 \right] \leq \frac{16 M_f^2}{216 M_f^2} + 5 M_f.
\]

where \( a_1(\alpha) - a_3(\alpha) \) are defined in (27).

Let

\[
\alpha_k^i = \frac{\alpha_k}{\tau_i}, \quad \forall i \in S \quad \text{where} \quad \alpha_k \leq \frac{1}{216 M_f^2 + 5 M_f}. \tag{49}
\]

The above choice of \( \alpha_k \) satisfies the condition of Lemma C.4 and we have \( 54 M_f^2 \alpha_k^4 \leq \alpha_k^2 / 4 \). Hence, from Lemma C.4, we get

\[
\frac{16 M_f^2}{216 M_f^2} + 5 M_f \leq \frac{1}{4} \frac{\alpha_k^4}{\tau_i} \mathbb{E} \left[ \| \nabla f(x^k) \|^2 \right] + \frac{3 M_f^2 \alpha_k^2}{4} \mathbb{E} \left[ \| x^k_{i,\nu} - x^k \|^2 \right] + \mathbb{E} \left[ \| x^k_{i,\nu} - y^k \|^2 \right] + 3 b^2 \]

Thus, for \( \beta_k \), the first inequality uses (49) and the last inequality follows from (26a).

To guarantee the descent of \( \mathbb{W}^k \), the following constraints need to be satisfied

\[
\frac{L_f \alpha_k^2}{2} - \frac{M_f}{L_y} \left( L_y^2 \alpha_k^2 + \frac{L_y x \alpha_k^2}{4 M_f} \right) \geq 0, \tag{50}
\]

where the second line uses (27).

Further, substituting (26) in (48c) gives

\[
\left( \frac{25 M_f}{L_y} \left( \frac{3 M_f L_y \alpha_k}{2} + a_2(\alpha_k) \right) T \beta_k^2 \sigma_{g,1} + \frac{M_f}{L_y} \left( \frac{3 M_f L_y \alpha_k}{2} + a_2(\alpha_k) \right) \left( 1 - \frac{\beta_k \mu_g}{2} \right) \right) \mathbb{E} \left[ \| y^k - y^* \| \right] \leq 0. \tag{52}
\]
Substituting (50)–(52) into (48) gives
\[
\mathbb{E}[W^{k+1}] - \mathbb{E}[W^k] \leq -\frac{\alpha_k}{4} \mathbb{E}[\|\nabla f(x^k)\|^2]
+ \left(\frac{3}{2} \alpha_k + \frac{3}{4} \alpha_k^2\right) b^2
+ \left(\frac{L_f}{2} + \frac{1}{4} \alpha_k^2 + \frac{M_f}{L_y} a_3(\alpha_k)\right) \bar{\sigma}_f^2
+ \frac{25M_f}{L_y} \left(\frac{M_f}{4} \alpha_k^2 + \frac{3M_f L_y a_k}{2} + a_2(\alpha_k)\right) T \beta_k^2 \sigma_{g,1}^2
+ \frac{M_f}{L_y} \left(\frac{M_f}{4} \alpha_k^2 + \frac{3M_f L_y a_k}{2} + a_2(\alpha_k)\right) \left(1 - \frac{\beta_k \mu_g}{2}\right) \mathbb{E}[\|y^k - y^*(x^k)\|^2].
\] (53a)

Let \( \beta_k < \min\left(\frac{1}{6\ell_g}, 1\right) \). Then, we have \(\beta_k \mu_g / 2 < 1\). This together with (27) implies that for any \( \alpha_k > 0 \)
\[
\Rightarrow \left(1 + \frac{M_f L_y}{4} \alpha_k^2 + \frac{11M_f L_y a_k}{2} + \frac{\eta L_y \bar{D}_f^2 \alpha_k^2}{2}\right) \left(1 - \frac{\beta_k \mu_g}{2}\right)^T - 1 \leq 0,
\]
\[
\Rightarrow \exp\left(\frac{M_f L_y}{4} \alpha_k^2 + \frac{11M_f L_y a_k}{2} + \frac{\eta L_y \bar{D}_f^2 \alpha_k^2}{2}\right) \exp\left(\frac{-T \beta_k \mu_g}{2}\right) - 1 \leq 0,
\] (54)
\[
\Rightarrow \beta_k \geq \frac{11M_f L_y + \eta L_y \bar{D}_f^2 \alpha_k + \frac{M_f L_y a_k}{2}}{\mu_g} \cdot \frac{\alpha_k}{T}.
\]

From (49), (51) and (54), we select
\[
\alpha_k = \min\{\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3, \bar{\alpha}\}, \quad \bar{\alpha}_k = \frac{\beta \alpha_k}{T},
\] (55)
where
\[
\bar{\beta} := \frac{1}{\mu_g} \left(11M_f L_y + \eta L_y \bar{D}_f^2 \bar{\alpha}_1 + \frac{M_f L_y \bar{\alpha}_1}{2}\right),
\]
\[
\bar{\alpha}_1 := \frac{1}{2L_f + 4M_f L_y + \frac{2M_f L_y \eta}{L_y \eta}}, \quad \bar{\alpha}_2 := \frac{T}{8\ell_g \beta}, \quad \bar{\alpha}_3 := \frac{1}{216M_f^2 + 5M_f}.
\] (56)

With the above choice of stepsizes, (53) can be simplified as
\[
\mathbb{E}[W^{k+1}] - \mathbb{E}[W^k] \leq -\frac{\alpha_k}{4} \mathbb{E}[\|\nabla f(x^k)\|^2]
+ \left(\frac{3}{2} \alpha_k + \frac{3}{4} \alpha_k^2\right) b^2
+ \left(\frac{L_f + \frac{1}{4} \alpha_k^2 + \frac{M_f}{L_y} a_3(\alpha_k)}{2}\right) \bar{\sigma}_f^2
+ \frac{25M_f}{L_y} \left(\frac{M_f}{4} \alpha_k^2 + \frac{3M_f L_y a_k}{2} + a_2(\alpha_k)\right) T \beta_k^2 \sigma_{g,1}^2
\leq -\frac{\alpha_k}{4} \mathbb{E}[\|\nabla f(x^k)\|^2]
+ c_1 \alpha_k^2 \sigma_{g,1}^2
+ \left(\frac{3}{2} \alpha_k + \frac{3}{4} \alpha_k^2\right) b^2
+ c_2 \alpha_k^2 \sigma_f^2,
\] (57)

where the constants \( c_1 \) and \( c_2 \) are defined as
\[
c_1 = \frac{25M_f}{L_y} \left(1 + \frac{11M_f L_y \bar{\alpha}_1}{2} + \left(\frac{M_f L_y + 2\eta L_y \bar{D}_f^2}{4}\right) \bar{\alpha}_1^2\right) \frac{\beta^2}{T},
\]
\[
c_2 = \frac{L_f + \frac{1}{4} \alpha_k^2}{2} + M_f L_y + \frac{L_y M_f}{4\eta L_y}.
\] (58)
Then telescoping gives
\[
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[[\nabla f(x^k)]] \leq \frac{4}{\sum_{k=0}^{K-1} \alpha_k} \left( \Delta_w + \sum_{k=0}^{K-1} \frac{3}{2} \left( \alpha_k + \frac{\alpha_k^2}{2} \right) b^2 + c_1 \alpha_k^2 \sigma^2_{g,1} + c_2 \alpha_k^2 \sigma^2_f \right)
\]
\[
\leq \frac{4 \Delta_w}{\min\{\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3\}} + \frac{4 \Delta_w}{\bar{\alpha} \sqrt{K}} + 6 \left( 1 + \frac{\bar{\alpha}}{2 \sqrt{K}} \right) b^2 + \frac{4c_1 \bar{\alpha}}{\sqrt{K}} \sigma^2_{g,1} + \frac{4c_2 \bar{\alpha}}{\sqrt{K}} \sigma^2_f
\]
(59)
\[= \mathcal{O}\left( \min\{\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3\} K + \bar{\alpha} \max(\sigma^2_{g,1}, \sigma^2_{g,2}, \sigma^2_f) + b^2 \right),\]
where \( \Delta_w := W^0 - \mathbb{E}[W^K] \).
\[\square\]

C.5. Proof of Corollary 3.1

Proof. Let \( \eta = \frac{M_i}{T_w} = \mathcal{O}(\kappa_g) \) in (58). It follows from (18), (56), and (58) that
\[
\bar{\alpha}_1 = \mathcal{O}(\kappa_g^{-3}), \quad \bar{\alpha}_2 = \mathcal{O}(T \kappa_g^{-3}), \quad \bar{\alpha}_3 = \mathcal{O}(\kappa_g^{-4}), \quad c_1 = \mathcal{O}(\kappa_g^0/T), \quad c_2 = \mathcal{O}(\kappa_g^3).
\]
(60)
Further, \( \mathcal{N} = \mathcal{O}(\kappa_g \log K) \) gives \( b = \frac{1}{\kappa_g \sqrt{K}} \). Now, if we select \( \bar{\alpha} = \mathcal{O}(\kappa_g^{-2.5}) \) and \( T = \mathcal{O}(\kappa_g^4) \), Eq. (59) gives
\[
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[[\nabla f(x^k)]] = \mathcal{O}\left( \frac{\kappa_g^4}{K} + \frac{\kappa_g^{2.5}}{\sqrt{K}} \right).
\]
To achieve \( \varepsilon \)-optimal solution, we need \( K = \mathcal{O}(\kappa_g^{2.5} \varepsilon^{-2}) \), and the samples in \( \xi \) and \( \zeta \) are \( \mathcal{O}(\kappa_g^5 \varepsilon^{-2}) \) and \( \mathcal{O}(\kappa_g^9 \varepsilon^{-2}) \), respectively.
\[\square\]

D. Proof for Federated Minimax Optimization

Note that the minimax optimization problem (2) has the following bilevel form
\[
\begin{align*}
\min_{x \in \mathbb{R}^d} & \quad f(x) = \frac{1}{m} \sum_{i=1}^{m} f_i(x, y^*(x)) \\
\text{subj. to} & \quad y^*(x) = \arg\min_{y \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1}^{m} f_i(x, y). \tag{61a}
\end{align*}
\]

Here,
\[
f_i(x, y) = \mathbb{E}_{\xi \sim C}[f_i(x, y; \xi)] \tag{61b}
\]
is the loss functions of the \( i \)-th client.

In this case, the hypergradient of (61) is
\[
\nabla f_i(x) = \nabla_x f_i(x, y^*(x)) + \nabla_x y^*(x)^{\top} \nabla_y f_i(x, y^*(x)) = \nabla_x f_i(x, y^*(x)),
\]
(62)
where the second equality follows from the optimality condition of the inner problem, i.e., \( \nabla_y f(x, y^*(x)) = 0 \).

For each \( i \in S \), we can approximate \( \nabla f_i(x) \) on a vector \( y \) in place of \( y^*(x) \), denoted as \( \nabla f_i(x, y) := \nabla_x f_i(x, y) \).
We also note that in the minimax case \( h_i \) is an unbiased estimator of \( \nabla f_i(x, y) \). Thus, \( b = 0 \). Therefore, we can apply \textbf{FEDNest} using
\[
q_{i,\nu} = -\nabla_y f_i(x, y_{i,\nu}; \xi_{i,\nu}) + \nabla_y f_i(x, y; \xi_{i,\nu}) - \frac{1}{m} \sum_{i=1}^{m} \nabla_y f_i(x, y; \xi),
\]
\[
h_{i,\nu} = \nabla_x f_i(x_{i,\nu}, y^*; \xi_{i,\nu}) - \nabla_x f_i(x, y^*; \xi) + \frac{1}{m} \sum_{i=1}^{m} \nabla_x f_i(x, y^*; \xi),
\]
(63)
D.1. Supporting Lemmas

Let \( z = (x, y) \in \mathbb{R}^{d_1 + d_2} \). We make the following assumptions that are counterparts of Assumptions A and B.

**Assumption E.** For all \( i \in [m] \):

(E1) \( f_i(z), \nabla f_i(z), \nabla^2 f_i(z) \) are respectively \( \ell_{f,0}, \ell_{f,1}, \ell_{f,2} \)-Lipschitz continuous; and

(E2) \( f_i(x, y) \) is \( \mu_f \)-strongly convex in \( y \) for any fixed \( x \in \mathbb{R}^{d_1} \).

We use \( \kappa_f = \ell_{f,1}/\mu_f \) to denote the condition number of the inner objective with respect to \( y \).

**Assumption F.** For all \( i \in [m] \):

(F1) \( \nabla f_i(z; \xi) \) is unbiased estimators of \( \nabla f_i(z) \); and

(F2) Its variance is bounded, i.e., \( \mathbb{E}_{\xi}[\|\nabla f_i(z; \xi) - \nabla f_i(z)\|^2] \leq \sigma_f^2, \) for some \( \sigma_f^2 \).

In the following, we re-derive Lemma C.1 for the finite-sum minimax problem (61).

**Lemma D.1.** Under Assumptions E and F, we have \( h_i(x, y) = \nabla f_i(x, y) \) for all \( i \in S \) and (17a)–(17g) hold with

\[
L_{yz} = \frac{\ell_{f,2} + \ell_{f,2}L_y}{\mu_f} + \frac{\ell_{f,1}(\ell_{f,2} + \ell_{f,2}L_y)}{\mu_f^2} = O(\kappa_f^3),
\]

\[
M_f = \ell_{f,1} = O(1), \quad L_f = (\ell_{f,1} + \ell_{f,1}^2/\mu_f) = O(\kappa_f),
\]

\[
L_y = \frac{\ell_{f,1}}{\mu_f} = O(\kappa_f), \quad \hat{\sigma}_f^2 = \sigma_f^2, \quad \hat{D}_f^2 = \ell_{f,0} + \sigma_f^2,
\]

where \( \ell_{f,0}, \ell_{f,1}, \ell_{f,2}, \mu_f, \) and \( \sigma_f \) are given in Assumptions E and F.

D.2. Proof of Corollary 3.2

**Proof.** Let \( \eta = 1 \). From (55) and (56), we have

\[
\alpha_k = \min\left\{ \tilde{\alpha}_1, \tilde{\alpha}_2, \tilde{\alpha}_3, \frac{\tilde{\alpha}}{\sqrt{K}} \right\}, \quad \beta_k = \frac{\tilde{\beta}\alpha_k}{T},
\]

where

\[
\tilde{\beta} = \frac{1}{L_g} \left( 11\ell_{f,1}L_y + L_{yz}\hat{D}_f^2\tilde{\alpha}_1 + \frac{\ell_{f,1}L_y\tilde{\alpha}_1}{2} \right),
\]

\[
\tilde{\alpha}_1 = \frac{1}{2L_f + 4\ell_{f,1}L_y + \frac{4\ell_{f,1}L_y}{L_y}}, \quad \tilde{\alpha}_2 = \frac{T}{8L_{y,1}\tilde{\beta}}, \quad \tilde{\alpha}_3 = \frac{1}{216\ell_{f,1}^2 + 5\ell_{f,1}}.
\]

Using the above choice of stepsizes, (59) reduces to

\[
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[\|\nabla f(x^k)\|^2] \leq \frac{4\Delta_w}{K \min\{\tilde{\alpha}_1, \tilde{\alpha}_2, \tilde{\alpha}_3\}} + \frac{4\Delta_w}{\tilde{\alpha}\sqrt{K}} + \frac{4(c_1 + c_2)\tilde{\alpha}}{\sqrt{K}} \sigma_f^2,
\]

where \( \Delta_w = W^0 - \mathbb{E}[W^K] \),

\[
c_1 = \frac{25\ell_{f,1}}{L_y} \left( 1 + \frac{11\ell_{f,1}L_y\tilde{\alpha}_1}{2} + \frac{(\ell_{f,1}L_y + 2L_{yz}\hat{D}_f^2)}{4}\tilde{\alpha}_1^2 \right) \tilde{\beta}^2 \frac{1}{T},
\]

\[
c_2 = \frac{L_f + \frac{1}{2}}{2} + \ell_{f,1}L_y + \frac{L_{yz}\ell_{f,1}}{4L_y},
\]

\[
c_3 = \frac{125\ell_{f,1}}{L_y} \left( 1 + \frac{11\ell_{f,1}L_y\tilde{\alpha}_1}{2} + \frac{(\ell_{f,1}L_y + 2L_{yz}\hat{D}_f^2)}{4}\tilde{\alpha}_1^2 \right) \tilde{\beta}^2 \frac{1}{T}.
\]
Let $\tilde{\alpha} = O(\kappa_f^{-1})$. Since by our assumption, $T = O(\kappa_f)$, it follows from (64) and (73) that
\begin{equation}
\tilde{\alpha}_1 = O(\kappa_f^{-2}), \quad \tilde{\alpha}_2 = O(\kappa_f^{-1}), \quad \tilde{\alpha}_3 = O(1), \quad c_1 = O(\kappa_f^2), \quad c_2 = O(\kappa_f^2).
\end{equation}
(68)

Substituting (68) in (66) and (67) gives
\begin{equation}
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[\|\nabla f(x^k)\|^2] = O \left( \frac{\kappa_f^2}{K} + \frac{\kappa_f}{\sqrt{K}} \right).
\end{equation}
(69)

To achieve $\varepsilon$-accuracy, we need $K = O(\kappa_f^2 \varepsilon^{-2})$.

**E. Proof for Federated Compositional Optimization**

Note that in the stochastic compositional problem (3), the inner function $f_i(x, y; \xi) = f_i(y; \xi)$ for all $i \in S$, and the outer function is $g_i(x, y; \xi) = \frac{1}{2}\|y - r_i(x; \xi)\|^2$, for all $i \in S$. In this case, we have
\begin{equation}
\nabla_y g_i(x, y) = y_i - r_i(x; \xi), \quad \nabla_{yy} g(x, y; \xi) = I_{d_2 \times d_2}, \quad \text{and} \quad \nabla_{xy} g(x, y; \xi) = -\frac{1}{m} \sum_{i=1}^{m} \nabla r_i(x; \xi)^\top.
\end{equation}
(70)

Hence, the hypergradient of (3) has the following form
\begin{equation}
\nabla f_i(x) = \nabla_x f_i(y^*(x)) - \nabla_{yy} g(x, y; \xi)[\nabla_{yy} g(x, y; \xi)]^{-1} \nabla_y f_i(y^*(x)) = \left( \frac{1}{m} \sum_{i=1}^{m} \nabla r_i(x) \right)^\top \nabla_y f_i(y^*(x)).
\end{equation}
(71)

We can obtain an approximate gradient $\nabla f_i(x)$ by replacing $y^*(x)$ with $y$, that is $\nabla f_i(x, y) = \left( \frac{1}{m} \sum_{i=1}^{m} \nabla r_i(x) \right)^\top \nabla_y f_i(y)$. It should be mentioned that in the compositional case $b = 0$. Thus, we can apply FedNest and LFedNest using the above gradient approximations.

**E.1. Supporting Lemmas**

Let $z = (x, y) \in \mathbb{R}^{d_1 + d_2}$. We make the following assumptions that are counterparts of Assumptions A and B.

**Assumption G.** For all $i \in [m]$, $f_i(z), r_i(z), \nabla r_i(z)$ are respectively $\ell_{f, \epsilon}, \ell_{r, \epsilon}, \ell_{r, \epsilon}$-Lipschitz continuous.

**Assumption H.** For all $i \in [m]$:

(H1) $\nabla f_i(z; \xi), r_i(x; \xi), \nabla r_i(x; \xi)$ are unbiased estimators of $\nabla f_i(z), r_i(x)$, and $\nabla r_i(x)$.

(H2) Their variances are bounded, i.e., $\mathbb{E}_\xi[\|\nabla f_i(z; \xi) - \nabla f_i(z)\|^2] \leq \sigma_f^2$, $\mathbb{E}_\xi[\|r_i(z; \xi) - r_i(z)\|^2] \leq \sigma_r^2$, and $\mathbb{E}_\xi[\|\nabla r_i(z; \xi) - \nabla r_i(z)\|^2] \leq \sigma_r^2$.

The following lemma is the counterpart of Lemma C.1. The proof is similar to (Chen et al., 2021a, Lemma 7).

**Lemma E.1.** Under Assumptions G and H, we have $\tilde{h}_i(x, y) = \nabla f_i(x, y)$ for all $i \in S$, and (17a)–(17g) hold with
\begin{equation}
M_f = \ell_{r, \epsilon} \ell_{f, 1}, \quad L_g = \ell_{r, \epsilon}, \quad L_f = \ell_{r, \epsilon} \ell_{f, 1} + \ell_{f, \epsilon} \ell_{r, 1}, \quad L_{yx} = \ell_{r, 1}, \quad \tilde{\sigma}_f^2 = \ell_{r, \epsilon}^2 \sigma_f^2 + (\ell_{f, \epsilon}^2 + \sigma_f^2) \sigma_r^2, \quad \tilde{D}_f^2 = (\ell_{f, \epsilon}^2 + \sigma_f^2) (\ell_{r, \epsilon}^2 + \sigma_r^2).
\end{equation}
(72)

**E.2. Proof of Corollary 3.3**

**Proof.** By our assumption $T = 1$. Let $\bar{\alpha} = 1$ and $\eta = 1/L_{yx}$. From (55) and (56), we obtain
\begin{equation}
\alpha_k = \min \left\{ \bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3, \frac{1}{\sqrt{K}} \right\}, \quad \beta_k = \bar{\beta}\alpha_k,
\end{equation}
(73a)
\[ \hat{\beta} = \frac{1}{\mu_g} \left( 11\ell_{f,1}\ell_{r,0}^2 + \bar{D}_f^2 \hat{\alpha}_1 + \frac{\ell_{f,1}\ell_{r,0}^2 \hat{\alpha}_1}{2} \right), \]

\[ \tilde{\alpha}_1 = \frac{1}{2\ell_{f,0}\ell_{r,1} + 6\ell_{f,1}\ell_{r,0}^2 + 2\ell_{f,1}\ell_{r,1}^2}, \quad \tilde{\alpha}_2 = \frac{1}{8\ell_{r,0}\beta}, \quad \tilde{\alpha}_3 = \frac{1}{216(\ell_{r,0}\ell_{f,1})^2 + 5\ell_{r,0}\ell_{f,1}}. \] (73b)

Then, using (59), we obtain

\[ \frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \| \nabla f(x^k) \|^2 \right] = O \left( \frac{1}{\sqrt{K}} \right). \] (74)

This completes the proof. \( \square \)

**F. Proof for Federated Single-Level Optimization**

Next, we re-derive Lemmas C.2 and C.4 for single-level nonconvex FL under Assumptions C and D.

**Lemma F.1** (Counterpart of Lemma C.2). Suppose Assumptions C and D hold. Further, assume \( \tau_i \geq 1 \) and \( \alpha_i = \alpha / \tau_i, \forall i \in S \) for some positive constant \( \alpha \). Then, \( \text{FedOut} \) guarantees:

\[
\begin{align*}
\mathbb{E} \left[ f(x^+) \right] - \mathbb{E} \left[ f(x) \right] & \leq -\frac{\alpha}{2} (1 - \alpha L_f) \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \nabla f_i(x_{i,\nu}) \right\|^2 \right] \\
& \quad - \frac{\alpha}{2} \mathbb{E} \left[ \| \nabla f(x) \|^2 \right] + \frac{\alpha L_f^2}{2m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \mathbb{E} \left[ \| x_{i,\nu} - x \|^2 \right] + \frac{\alpha^2 L_f}{2} \sigma_f^2.
\end{align*}
\] (75)

**Proof.** By applying Algorithm 2 to the single-level optimization problem (13), we have

\[ x_{i,0} = x \quad \forall i \in S, \quad x^+ = x - \frac{1}{m} \sum_{i=1}^{m} \alpha_i \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}). \]

where

\[ h_i(x_{i,\nu}) := \nabla_x f_i(x_{i,\nu}; \xi_{i,\nu}) - \nabla_x f_i(x; \xi_{i,\nu}) + \frac{1}{m} \sum_{i=1}^{m} \nabla_x f_i(x; \xi_i). \]

This together with Assumption C implies that

\[
\begin{align*}
\mathbb{E} \left[ f(x^+) \right] - \mathbb{E} \left[ f(x) \right] & \leq \mathbb{E} \left[ (x^+ - x, \nabla f(x)) \right] + \frac{L_f}{2} \mathbb{E} \left[ \| x^+ - x \|^2 \right] \\
& = -\mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \alpha_i \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}), \nabla f(x) \right\|^2 \right] \\
& \quad + \frac{L_f}{2} \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \alpha_i \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}) \right\|^2 \right] \quad (76)
\end{align*}
\]
For the first term on the RHS of (76), we obtain
\[
-\mathbb{E} \left[ \frac{1}{m} \sum_{i=1}^{m} \alpha_i \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, \nabla f(x)) \right] = -\mathbb{E} \left[ \frac{1}{m} \sum_{i=1}^{m} \alpha_i \sum_{\nu=0}^{\tau_i-1} \mathbb{E}[(h_i(x_{i,\nu}), \nabla f(x)) | \mathcal{F}_{i,\nu-1}] \right] \\
= -\frac{\alpha}{2} \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} \nabla f_i(x_{i,\nu}) \right\|^2 \right] - \frac{\alpha}{2} \mathbb{E} \left[ \left\| \nabla f(x) \right\|^2 \right] \\
+ \frac{\alpha}{2} \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} \nabla f_i(x_{i,\nu}) - \nabla f(x) \right\|^2 \right], \quad (77)
\]
where the first equality follows from the law of total expectation and the last inequality is obtained from Assumption C.

For the second term on the RHS of (76), Assumption D gives
\[
\mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \alpha_i \sum_{\nu=0}^{\tau_i-1} h_i(x_{i,\nu}, y^+) \right\|^2 \right] = \alpha^2 \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} \left( h_i(x_{i,\nu}) - \nabla f_i(x_{i,\nu}) + \nabla f_i(x_{i,\nu}) \right) \right\|^2 \right] \\
\leq \alpha^2 \mathbb{E} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \sum_{\nu=0}^{\tau_i-1} \nabla f_i(x_{i,\nu}) \right\|^2 \right] + \alpha^2 \sigma_j^2. \quad (78)
\]
Plugging (78) and (77) into (76) gives the desired result. □

**Lemma F.2** (Counterpart of Lemma C.4). Suppose Assumptions C and D hold. Further, assume \( \tau_i \geq 1 \) and \( \alpha_i = \alpha / \tau_i, \forall i \in \mathcal{S}, \) where \( \alpha \leq 1 / (3L_f) \). Then, for all \( \nu \in \{0, \ldots, \tau_i - 1\} \), FeDOut gives
\[
\mathbb{E} \left[ \left\| x_{i,\nu} - x \right\|^2 \right] \leq 12 \tau_i^2 \alpha^2 \mathbb{E} \left[ \left\| \nabla f(x) \right\|^2 \right] + 27 \tau_i \alpha^2 \sigma_j^2. \quad (79)
\]

**Proof.** The result trivially holds for \( \tau_i = 1 \). Similar to what is done in the proof of Lemma C.4, let \( \tau_i > 1 \) and define
\[
\begin{align*}
\nu_{i,\nu} &:= \nabla f_i(x_{i,\nu}) - \nabla f_i(x) + \nabla f(x), \\
w_{i,\nu} &:= h_i(x_{i,\nu}) - \nabla f_i(x_{i,\nu}) + \nabla f_i(x) - h_i(x) + h(x) - \nabla f(x).
\end{align*}
\]
where \( h_i(x) = \nabla_x f_i(x; \xi_{i,\nu}) \) and \( h(x) = 1/m \sum_{i=1}^{m} \nabla_x f_i(x; \xi_i) \).

From Algorithm 2, for each \( i \in \mathcal{S} \), and \( \forall \nu \in \{0, \ldots, \tau_i - 1\} \), we obtain
\[
\begin{align*}
x_{i,\nu+1} - x &= x_{i,\nu} - x - \alpha_i (h_i(x_{i,\nu}) - h_i(x) + h(x)) \\
&= x_{i,\nu} - x - \alpha_i (\nu_{i,\nu} + w_{i,\nu}),
\end{align*}
\]
which implies that
\[
\mathbb{E} \left[ \left\| x_{i,\nu+1} - x \right\|^2 \right] = \mathbb{E} \left[ \left\| x_{i,\nu} - x - \alpha_i \nu_{i,\nu} \right\|^2 \right] + \alpha_i^2 \mathbb{E} \left[ \left\| w_{i,\nu} \right\|^2 \right] \\
- 2 \mathbb{E} \left[ \left\langle x_{i,\nu} - x - \alpha_i \nu_{i,\nu}, \alpha_i \nu_{i,\nu} \right\rangle | \mathcal{F}_{i,\nu-1} \right] \\
= \mathbb{E} \left[ \left\| x_{i,\nu} - x - \alpha_i \nu_{i,\nu} \right\|^2 \right] + \alpha_i^2 \mathbb{E} \left[ \left\| w_{i,\nu} \right\|^2 \right]. \quad (81)
\]
Here, the last equality uses Lemma G.3 since \( \mathbb{E}[w_{i,\nu} | \mathcal{F}_{i,\nu-1}] = 0 \).
From Assumption D and Lemma G.1, for $w_{i,\nu}$ defined in (80), we have
\[
E[\|w_{i,\nu}\|^2] \leq 3E[\|h_i(x_{i,\nu}) - \nabla f_i(x_{i,\nu})\|^2 + \|\nabla f_i(x) - h_i(x)\|^2 + \|h(x) - \nabla f(x)\|^2] 
\leq 9\sigma_f^2. \tag{82}
\]
Substituting (82) into (81), we get
\[
E[\|x_{i,\nu} - x - \alpha_i v_{i,\nu}\|^2] \leq \left(1 + \frac{1}{2\tau_i - 1}\right)E[\|x_{i,\nu} - x\|^2] + 2\tau_i\alpha_i^2E[\|v_{i,\nu}\|^2] + 9\alpha_i^2\sigma_f^2 
\leq \left(1 + \frac{1}{2\tau_i - 1} + 4\tau_i\alpha_i^2L_f^2\right)E[\|x_{i,\nu} - x\|^2] + 4\tau_i\alpha_i^2E[\|\nabla f(x)\|^2] + 9\alpha_i^2\sigma_f^2 \tag{83}
\]
Here, the first inequality follows from Lemma G.2; the second inequality uses Assumption C and Lemma G.1; and the last inequality follows by noting $\alpha_i = \alpha/\tau_i, \forall i \in S$ and $\alpha \leq 1/(3L_f)$.

Now, iterating equation (83) and using $x_{i,0} = x, \forall i \in S$, we obtain
\[
E[\|x_{i,\nu} - x\|^2] \leq (4\tau_i\alpha_i^2E[\|\nabla f(x)\|^2] + 9\alpha_i^2\sigma_f^2) \sum_{j=0}^{\nu-1} \left(1 + \frac{1}{\tau_i - 1}\right)^j 
\leq 12\tau_i^2\alpha_i^2E[\|\nabla f(x)\|^2] + 27\tau_i\alpha_i^2\sigma_f^2, \tag{84}
\]
where the second inequality uses (45). This completes the proof. \hfill \Box

F.1. Proof of Theorem 3.2

\textbf{Proof.} Let $\bar{\alpha}_1 := 1/(3L_f(1 + 8L_f))$. Note that by our assumption $\alpha_k \leq \bar{\alpha}_1$. Hence, the stepsizes $\alpha_k$ satisfies the condition of Lemma F.2, and we have $6L_f^2\alpha_k^2 \leq \alpha_k^2/4$. This together with Lemmas F.1 and F.2 gives
\[
E[f(x^{k+1})] - E[f(x^k)] 
\leq -\frac{\alpha_k}{2} E[\|\nabla f(x^k)\|^2] + \frac{L_f^2\alpha_k}{2m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} E[\|x_{i,\nu}^k - x^k\|^2] 
- \frac{\alpha_k}{2}(1 - \alpha_k L_f) E \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} \nabla f_i(x_{i,\nu}^k) \right\|^2 \right] + \frac{\alpha_k^2 L_f^2}{2}\sigma_f^2 
\leq -\frac{\alpha_k}{2} E[\|\nabla f(x^k)\|^2] + \frac{L_f^2\alpha_k}{2m} \sum_{i=1}^{m} \frac{1}{\tau_i} \sum_{\nu=0}^{\tau_i-1} E[\|x_{i,\nu}^k - x^k\|^2] + \frac{\alpha_k^2 L_f^2}{2}\sigma_f^2 
\leq -\frac{\alpha_k}{2} E[\|\nabla f(x^k)\|^2] + 6L_f^2\alpha_k^3 E[\|\nabla f(x^k)\|^2] + \left(\frac{27}{2}\alpha_k^2 L_f^2 + \frac{\alpha_k^2 L_f^2}{2}\sigma_f^2 \right) \tag{85}
\leq -\frac{\alpha_k}{4} E[\|\nabla f(x^k)\|^2] + (4 + L_f)\alpha_k^2\sigma_f^2,
\]
where the second and last inequalities follow from (14).

Summing (85) over $k$ and using our choice of stepsize in (14), we obtain
\[
\frac{1}{K} \sum_{k=0}^{K-1} E[\|\nabla f(x^k)\|^2] \leq \frac{4\Delta_f}{K} \cdot \min \left\{ \frac{1}{\bar{\alpha}_1}, \frac{\sqrt{K}}{\bar{\alpha}} \right\} + 4(4 + L_f)\sigma_f^2 \cdot \frac{\bar{\alpha}}{\sqrt{K}} 
\leq \frac{4\Delta_f}{\bar{\alpha}_1 K} + \left(\frac{4\Delta_f}{\bar{\alpha}} + 4(4 + L_f)\bar{\alpha}\sigma_f^2 \right) \frac{1}{\sqrt{K}}, \tag{86}
\]
where $\Delta_f = f(x^0) - E[f(x^K)]$. \hfill \Box
G. Other Technical Lemmas

We collect additional technical lemmas in this section.

**Lemma G.1.** For any set of vectors \( \{x_i\}_{i=1}^m \) with \( x_i \in \mathbb{R}^d \), we have

\[
\left\| \sum_{i=1}^m x_i \right\|^2 \leq m \sum_{i=1}^m \|x_i\|^2 .
\]

(87)

**Lemma G.2.** For any \( x, y \in \mathbb{R}^d \), the following holds for any \( c > 0 \):

\[
\|x + y\|^2 \leq (1 + c)\|x\|^2 + \left(1 + \frac{1}{c}\right)\|y\|^2 .
\]

(88)

**Lemma G.3.** For any set of independent, mean zero random variables \( \{x_i\}_{i=1}^m \) with \( x_i \in \mathbb{R}^d \), we have

\[
\mathbb{E}\left[ \sum_{i=1}^m \|x_i\|^2 \right] = \sum_{i=1}^m \mathbb{E}\left[ \|x_i\|^2 \right] .
\]

(89)

H. Additional Experimental Results

In this section, we first provide the detailed parameters in Section 4 and then discuss more experiments. In Section 4, our federated algorithm implementation is based on (Ji, 2018), both hyper-representation and loss function tuning use batch size 64 and Neumann series parameter \( N = 5 \). We conduct 5 SGD/SVRG epoch of local updates in FEDNN and \( \tau = 1 \) in FEDOUT. In FEDNEST, we use \( T = 1 \), have 100 clients in total, and 10 clients are selected in each FEDNEST epoch.

![Figure 5: Hyper representation experiment comparing LFEDNEST, LFEDNESTSVRG and LFEDNEST-NONALT on non-i.i.d dataset. The number in parentheses corresponds to communication rounds shown in Table 2.](image)

**H.1. The effect of the alternating between inner and outer global variables**

In our addition experiments, we investigate the effect of the alternating between inner and outer global variables \( x \) and \( y \). We use LFEDNEST-NONALT to denote the training where each client updates their local \( y_i \) and then update local \( x_i \) w.r.t. local \( y_i \) for all \( i \in S \). Hence, the nested optimization is performed locally (within the clients) and the joint variable \([x_i, y_i]\) is communicated with the server. One can notice that only one communication is conducted when server update global \( x \) and \( y \) by aggregating all \( x_i \) and \( y_i \).
As illustrated in Figure 5, the test accuracy of LFEDNEST-NONALT remains around 80%, but both standard LFEDNEST and LFEDNEST_SVRG achieves better performance. Here, the number of inner iterations is set to $T = 1$. The performance boost reveals the necessity of both averaging and SVRG in FedINN, where the extra communication makes clients more consistent.

H.2. The effect of the learning rate and the global inverse Hessian

Figure 6 shows that on non-i.i.d. dataset, both SVRG and FedOUT have the effect of stabilizing the training. Here, we set $T = 1$ and $N = 5$. As we observe in (a)-(d), where the learning rate decreases, the algorithms with more communications are easier to achieve convergence. We note that LFEDNEST successfully converges in (d) with a very small learning rate. In contrast, in (a), FedNEST (using the global inverse Hessian) achieves better test accuracy in the same communication round with a larger learning rate.