Alternating Implicit Projected SGD and Its Efficient Variants for Equality-constrained Bilevel Optimization

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Abstract
Stochastic bilevel optimization, which captures the inherent nested structure of machine learning problems, is gaining popularity in many recent applications. Existing works on bilevel optimization mostly consider either unconstrained problems or constrained upper-level problems. This paper considers the stochastic bilevel optimization problems with equality constraints both in the upper and lower levels. By leveraging the special structure of the equality constraints problem, the paper first presents an alternating implicit projected SGD approach and establishes the $\tilde{O}(\epsilon^{-2})$ sample complexity that matches the state-of-the-art complexity of ALSET [8] for unconstrained bilevel problems. To further save the cost of projection, the paper presents two alternating implicit projection-efficient SGD approaches, where one algorithm enjoys the $\tilde{O}(\epsilon^{-1.5}/T^{3/4})$ upper-level and $\tilde{O}(\epsilon^{-1}/T)$ lower-level projection complexity with $O(T)$ lower-level batch size, and the other one enjoys $\tilde{O}(\epsilon^{-1.5})$ upper-level and lower-level projection complexity with $O(1)$ batch size. Application to federated bilevel optimization has been presented to showcase the empirical performance of our algorithms. Our results demonstrate that equality-constrained bilevel optimization with strongly-convex lower-level problems can be solved as efficiently as stochastic single-level optimization problems.

1 Introduction
Projected stochastic gradient descent (SGD) is a fundamental approach to solving large-scale constrained single-level machine learning problems. Specifically, to minimize $E_\xi [L(x; \xi)]$ over a given convex set $\mathcal{X}$, it generates the sequence $x^{k+1} = \text{Proj}_{\mathcal{X}}(x^k - \alpha \nabla L(x^k; \xi^k))$, where $\alpha > 0$ is the stepsize and $\nabla L(x^k; \xi^k)$ is a stochastic gradient estimate of $E_\xi [L(x^k; \xi)]$. If $E_\xi [L(x; \xi)]$ is non-convex, projected SGD requires a sample complexity of $O(\epsilon^{-2})$ with $O(1/\epsilon)$ batch size [25]. The requirement of $O(1/\epsilon)$ batch size has been later relaxed [14] using the Moreau envelope technique, and its convergence rate matches that of vanilla SGD.

However, recent machine learning applications often go beyond the single-level structure, including hyperparameter optimization [19, 47], meta-learning, [18] reinforcement learning, [56] and neural architecture search [40]. While the nonasymptotic analysis of the alternating implicit SGD for

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unconstrained bilevel optimization with strongly convex and smooth lower-level problems was well-understood \[8, 24, 29, 32, 37\], to the best of our knowledge, the finite-time guarantee of alternating implicit projected SGD on bilevel problems with both upper-level (UL) and lower-level (LL) constraints have not been investigated yet. In this context, a natural but important question is

*Can we establish the $\tilde{O}(e^{-2})$ sample complexity of alternating implicit projected SGD for a family of bilevel problems with both UL and LL constraints?*

We give an affirmative answer to this question for the following *stochastic bilevel optimization problems* with both UL and LL constraints, given by

\[
\begin{align}
\min_{x \in \mathcal{X}} \quad & F(x) \triangleq \mathbb{E}_\xi[f(x, y^*(x); \xi)] \quad \text{(upper)} \quad (1a) \\
\text{s.t.} \quad & y^*(x) \triangleq \arg\min_{y \in \mathcal{Y}(x)} \mathbb{E}_\phi[g(x, y; \phi)] \quad \text{(lower)} \quad (1b)
\end{align}
\]

where $\xi$ and $\phi$ are random variables, $\mathcal{X} = \{x \mid B x = e\} \subset \mathbb{R}^{d_x}$ and $\mathcal{Y}(x) = \{y \mid A y + h(x) = c\} \subset \mathbb{R}^{d_y}$ are closed convex set; $A \in \mathbb{R}^{m_y \times d_y}$, $B \in \mathbb{R}^{m_x \times d_x}$, $c \in \mathbb{R}^{m_y}$, $e \in \mathbb{R}^{m_x}$, $h : \mathbb{R}^{d_x} \rightarrow \mathbb{R}^{m_y}$; $A$ and $B$ are not necessarily full row or column rank and the coupling function $h$ can be nonlinear. In (1), the UL optimization problem depends on the solution of the LL optimization over $y$, and both the LL function and constraint set depend on the UL variable $x$. The equality-constrained bilevel problem (1) covers a wider class of applications than unconstrained bilevel optimization, such as distributed bilevel optimization \[57, 63\], hyperparameter optimization for optimal transport \[27, 46\], and the design of transportation networks \[1, 48\]. When $A = 0$, $B = 0$, $h = 0$, $c = 0$, $e = 0$, the problem (1) reduces to the unconstrained stochastic bilevel problem \[8, 9, 24, 29, 32, 35, 37\].

Generically speaking, to solve (1), alternating implicit projected SGD performs

\[
y^{k+1} = \text{Proj}_{\mathcal{Y}(x^k)} \left( y^k - \beta h^k_y \right) \quad \text{and} \quad x^{k+1} = \text{Proj}_{\mathcal{X}} \left( x^k - \beta h^k_x \right),
\]

where $h^k_y$ is an unbiased stochastic gradient estimator of $\mathbb{E}_\phi[g(x^k, y^k; \phi)]$, $h^k_x$ is a (possibly biased) stochastic gradient estimator of $F(x^k)$, and, $\alpha$ and $\beta$ are step sizes. An immediate difficulty in analyzing the stochastic methods for (1) is that $h^k_x$ is usually biased due to the inaccessibility of $y^*(x)$. Moreover, the bias is roughly proportional to the LL accuracy $\|y^{k+1} - y^*(x^k)\|$, but the latter is not ensured to be small enough after finite LL steps. Therefore, if we directly apply the existing analysis for nonconvex constrained single-level problems \[14\] to even merely UL constrained bilevel problems, it either leads to a suboptimal rate \[29\] or requires additional LL corrections \[9\], let alone coupled with LL constraints. Leveraging the smoothness of the projection to linear equality constraints, we establish the convergence of alternating implicit projected SGD comparable to the unconstrained case.

Despite its popularity, alternating implicit projected SGD is not suitable for scenarios where evaluating projections is expensive since it calls projections at each step. For the linear equality constraints in (1), although the projection onto the set of constraints has the analytical solution (See \[5\] or Appendix A), assessing it involves calculating the product of the projection matrix with a vector which is computationally costly when the projection matrix is high-rank. Even if the projection matrix is low-rank, it would also suffer from other bottlenecks. For example, in federated bilevel learning \[57\], projection is low-rank and simple as it amounts to averaging the gradients of all clients \[52\]. However, as the data is stored on the client side and clients are only able to communicate with the server, obtaining the projection suffers from extreme communication costs. Therefore, this inspires us to design a provable projection efficient algorithm for (1) beyond alternating implicit projected SGD.
1.1 Contributions

In this context, we consider bilevel optimization with equality constraints. We analyze the convergence rate for alternating implicit projected SGD, AiPOD for short, propose two projection efficient variants of AiPOD, and apply them to federated bilevel optimization. We summarize our contributions below.

C1) We provide the first nonasymptotic analysis of AiPOD for bilevel optimization with both UL and LL constraints and attain the $\tilde{O}(\epsilon^{-2})$ sample and iteration complexity to achieve $\epsilon$ stationary point of (1), which matches the complexity of alternating implicit SGD algorithm for the unconstrained bilevel problem [8].

C2) Leveraging the recent work Proxskip [50], we propose two efficient variants of AiPOD termed E-AiPOD and E2-AiPOD tailored to the setting where evaluating projection is costly. In the setting (1), E-AiPOD reduces the UL and LL projection complexity from $\tilde{O}(\epsilon^{-2})$ to $\tilde{O}(\epsilon^{-2}/T)$ and $\tilde{O}(\epsilon^{-1.5}/T^{2/3})$ with $O(T)$ LL batch size. In the setting (1) with $h(x) = 0$, E2-AiPOD reduces both the UL and LL projection complexity to $\tilde{O}(\epsilon^{-1.5})$ with $O(1)$ batch size.

C3) We show the implication of the proposed method in federated bilevel learning and provide improved communication complexity over the state-of-the-art work [57]. Experiments on numerical and federated examples are provided to verify our theoretical findings.

1.2 Technical challenges

We highlight the technical challenges for the theoretical analysis.

T1) The state-of-the-art analysis of unconstrained bilevel optimization [8, 24, 29, 32] relies on the smoothness of the implicit solution mapping $y^*(x)$. However, the well-known formula of $\nabla y^*(x)$ does not hold when LL problem has coupling constraints so that the smoothness of $y^*(x)$ is unexplored.

T2) The update of UL can be viewed as biased projected SGD but the bias of the gradient estimator leads to suboptimal rates in the general analysis of projected SGD [14] since we can not separate out a negative term to mitigate the LL bias.

T3) The Lyapunov function that is critical in analyzing the single-loop unconstrained bilevel optimization [8] is insufficient for the analysis of our projection-efficient variant E-AiPOD and E2-AiPOD due to the additional errors caused by skipping projection steps.

T4) Analysis for E2-AiPOD relies on the convergence of multiple coupling sequences, but the new implicit solution mapping generated by E2-AiPOD is not Lipschitz smooth, which prevents us from leveraging the recent advance in multi-sequence stochastic approximation [53].

1.3 Related works

To put our work in context, we review prior art from the following two categories. We summarize the comparison of our work with the closely related prior art in Table 1.
Unconstrained bilevel optimization. Bilevel optimization has a long history back to [6] and has inspired rich literature, e.g., [12, 54, 59, 64]. Later on, spurred by the advancement of hyperparameter optimization [20, 47] and meta-learning [18], bilevel optimization received more attention as a unified tool for problems with nested structures. With more use cases in large-scale machine learning, developing stochastic methods with finite-time guarantees has become the recent focus in the area of bilevel optimization. The interest in the nonasymptotic analysis of the stochastic bilevel optimization has been stimulated since a recent work [24] that tackles the bilevel setting where the LL objective is strongly convex and Lipschitz smooth. As $\nabla F(x)$ contains the Hessian inverse of the LL objective which is computationally expensive, it has emerged various numeric approximation methods including Neumann series approximation [24], unrolling differentiation [28], and conjugate gradient [32]; see comparisons in [33, 43]. In terms of the alternating implicit SGD algorithm, [8] achieved the $O(\epsilon^{-2})$ sample complexity, which matches the results for the single-level case. Beyond the alternating implicit SGD framework, [35, 62] incorporated variance reduction techniques to further accelerate the convergence, [37] has put forward a fully single-loop algorithm with UL variance reduction and achieved $O(\epsilon^{-2})$ sample complexity, and later on, [13] generalized this framework to allow global variance reduction for each level and further enhanced the convergence rate; see a recent survey for bilevel optimization [41]. Nevertheless, none of these attempts can solve (1) in the presence of both UL and LL constraints.

Constrained bilevel optimization. While the nonasymptotic convergence for various approaches in the unconstrained bilevel setting has been extensively studied in the literature, the nonasymptotic analysis of stochastic algorithms for constrained bilevel optimization problems is very limited. Some recent efforts have been devoted to tackling the constrained UL setting. [29] has established $O(\epsilon^{-2.5})$ rate of TTSA which applied SGD in LL update and projected SGD in UL update; [9] has achieved $O(\epsilon^{-2})$ convergence rate by adding additional corrections on LL update for the stochastic setting; [11] has proved the $O(\epsilon^{-1})$ convergence rate of the proximal accelerated gradient-based method for deterministic constrained UL problem under the Kurdyka-Łojasiewicz geometry. As for constrained LL problem, the vast majority of works focus on either asymptotic analysis, e.g., initialization auxiliary.
method [42], value function based approach [23]; or design aspects, e.g. optimality of bilevel problem [17, 65], reformulation [7, 16], and implicit differential properties [3, 4, 26]. The notable exception is a recent work [58], which solved linearly inequality constrained LL problem in a double-loop manner, i.e. update UL variable after attaining a sufficiently accurate LL solution. However, the overall iteration complexity has not been established therein.

2 AiPOD: Alternating Implicit Projected SGD for Bilevel Problems

In this section, we first introduce notations, present the algorithm and establish its convergence.

2.1 Preliminaries

For convenience, we define \( g(x,y) := \mathbb{E}_\phi [g(x,y; \phi)] \) and \( f(x,y) := \mathbb{E}_\xi [f(x,y; \xi)] \). We also define \( \nabla_{yy} g(x,y) \) as the Hessian of \( g \) with respect to \( y \) and denote

\[
\nabla_{xy} g(x,y) = \begin{bmatrix}
\frac{\partial^2}{\partial x \partial y_1} g(x,y) & \cdots & \frac{\partial^2}{\partial x \partial y_d} g(x,y) \\
\vdots & \ddots & \vdots \\
\frac{\partial^2}{\partial x_d \partial y_1} g(x,y) & \cdots & \frac{\partial^2}{\partial x_d \partial y_d} g(x,y)
\end{bmatrix}.
\]

We use \( \| \cdot \| \) to denote the \( \ell_2 \) norm for vectors and Frobenius norm for matrix. We also denote \( A^\dagger \) and \( B^\dagger \) as the Moore-Penrose inverse of \( A \) and \( B \) [31]. Moreover, we define \( P_x := I - B^\dagger B \) and \( P_y := I - A^\dagger A \) as the projection matrix over \( x \) and \( y \), and denote \( \|x\|_{P_x} := \sqrt{x^\top P_x x} \) and \( \|y\|_{P_y} := \sqrt{y^\top P_y y} \) as the \( P_x \) and \( P_y \) weighted Euclidean norm, respectively. We also let \( V_1 \) be the orthogonal basis of \( \text{Ran}(A^\top) := \{ A^\top y \} \) and \( V_2 \) be the orthogonal basis of \( \text{Ker}(A) := \{ y \mid Ay = 0 \} \).

The common convergence metric for constrained optimization is [25]

\[
\mathbb{E}[\| \lambda^{-1} (x - \text{Proj}_X (x - \lambda \nabla F(x))) \|_2^2]
\]  

for some \( \lambda > 0 \). In (1), since \( X \) contains only linear equality constraints, (3) can be simplified according to the following lemma, the proof of which will be deferred to Appendix A.

**Lemma 1.** For any \( x \in X := \{ x \mid Bx = e \} \) and any \( \lambda > 0 \), we have that

\[
\| \lambda^{-1} (x - \text{Proj}_X (x - \lambda \nabla F(x))) \|_2^2 = \| \nabla F(x) \|_{P_x}^2.
\]

Therefore, we have the following definition of the \( \epsilon \) stationary point.

**The \( \epsilon \) stationary point.** We define the \( \epsilon \) stationary point \( x \) for (1) as

\[
\mathbb{E}[\| \nabla F(x) \|_{P_x}^2] \leq \epsilon.
\]  

If \( B = 0 \), (4) is reduced to \( \mathbb{E}[\| \nabla F(x) \|_2^2] \leq \epsilon \), which is the standard stationary measure for unconstrained stochastic bilevel optimization settings [8, 24, 32].

2.2 The basic algorithm
In this section, we will introduce the basic version of AiPOD algorithm for (1), which updates $x$ and $y$ in an alternating implicit projected SGD manner.

At a given UL iteration $k$, we update $y^{k+1}$ by the output of the $S$ projected SGD steps for $g(x, y)$. With initialization $y^{k,0} = y^k$, we update

$$y^{k,s+1} = \text{Proj}_\mathcal{Y}(y^k - \beta \nabla g(x^k, y^{k,s}; \phi^{k,s}))$$

(5)

and set $y^{k+1} = y^{k,S}$. For UL, the gradient $\nabla F(x)$ can be calculated by the chain rule

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

(6)

Therefore, the implicit mapping $\nabla y^*(x)$ is essential to the UL update.

Without LL constraint, $\nabla y^*(x)$ can be derived from the LL optimality condition $\nabla_y g(x, y^*(x)) = 0$ as [24]

$$\nabla y^*(x) = -\nabla_y^{-1} g(x, y^*(x)) \nabla_{yx} g(x, y^*(x)).$$

(7)

We generalize it to the constrained LL setting and establish the implicit gradient for constrained LL in the following lemma, the proof of which is deferred to Appendix A.

Lemma 2. Define $V_2$ as the orthogonal basis of $\text{Ker}(A) := \{y \mid Ay = 0\}$. When $g(x, y)$ is twice differentiable and strongly convex over $y$, the implicit gradient $\nabla y^*(x)$ can be written as

$$\nabla y^*(x) = -V_2 (V_2^\top \nabla_{yx} g(x, y^*(x)) V_2) V_2^\top (\nabla_{yx} g(x, y^*(x)) - \nabla_{yy} g(x, y^*(x)) \hat{A}^\dagger \nabla h(x)),$$

$$- \hat{A}^\dagger \nabla h(x)$$

(8)

where $\hat{A}^\dagger$ is the Moore-Penrose inverse of $A$.

Compared with (7), the term $P_1$ in (8) can be roughly viewed as projecting $\nabla_{yx}^{-1} g(x, y^*(x))$ to $\text{Ker}(A)$; while $P_2$ accounts for the coupling constraints $Ay + h(x) = c$.

With similar spirits with the existing works [8, 24, 29], we obtain the UL gradient estimator $h_f^k$ at UL iteration $k$ by setting $x = x^k$, approximating $y^*(x^k)$ by $y^{k+1}$ in (6) and estimating $P_1$ by Neumann series. Formally, $h_f^k$ is defined as

$$h_f^k := \nabla_x f(x^k, y^{k+1}; \xi^k) + w^k$$

(9a)

with $w^k := \left\{-\nabla h(x^k) \hat{A}^\top + \left(\nabla h(x^k) \hat{A}^\top \nabla_{yy} g(x^k, y^{k+1}; \phi^{k}) - \nabla_{yx} g(x^k, y^{k+1}; \phi^{k})\right)\right\}$

$$\times V_2 \left[\frac{\tilde{c} N}{\ell_g, 1} \prod_{n=1}^{N'} \left(1 - \frac{\tilde{c}}{\ell_g, 1} V_2^\top \nabla_{yx} g(x^k, y^{k+1}; \phi^{k}) V_2\right) V_2^\top \nabla y f(x^k, y^{k+1}; \xi^k)\right]$$

(9b)

where $\tilde{c} \in (0, 1]$ is a given constant, $N'$ is drawn uniformly at random from $\{0, \ldots, N - 1\}$, and $\{\phi^{k}, \ldots, \phi^{k(N')}\}$ are i.i.d samples.

Afterward, we can update $x^{k+1}$ by projected SGD with estimator $h_f^k$ in (9a). The full AiPOD algorithm is summarized in Algorithm 1.

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**Algorithm 1** AiPOD for constrained bilevel problem

1. Initialization: $x^0, y^0$, stepsizes $\{\alpha, \beta\}$, the number of LL and UL rounds $\{S, K\}$, the number of $\phi$ samples $N$
2. for $k = 0$ to $K - 1$ do
   3. for $s = 0$ to $S - 1$ do ▷ Set $y^{k,0} = y^k$
      4. update $y^{k,s+1}$ by (5).
   5. end for ▷ Set $y^{k+1} = y^{k,S}$
   6. evaluate $w^k$ in (9b) and $h_f^k$ in (9a)
   7. update $x^{k+1} = \text{Proj}_\mathcal{X}(x^k - \alpha h_f^k)$
8. end for
2.3 Theoretical analysis

For the subsequent analysis, we make the following assumptions.

**Assumption 1.** Assume that $f, \nabla f, \nabla g, \nabla_{xy} g, \nabla_{yy} g, h$ and $\nabla h$ are Lipschitz continuous with $\ell_f, 0, \ell_g, 1, \ell_g, 2, \ell_h, 0$ and $\ell_h, 1$, respectively.

**Assumption 2.** For any fixed $x$, assume that $g(x,y)$ is $\mu_g$-strongly convex with respect to $y \in \mathbb{R}^{d_g}$.

**Assumption 3.** The stochastic estimators $\nabla f(x,y; \xi), \nabla g(x,y; \phi), \nabla_{xy} g(x,y; \phi)$ and $\nabla_{yy} g(x,y; \phi)$ are unbiased estimators of $\nabla f(x,y), \nabla g(x,y), \nabla_{xy} g(x,y)$ and $\nabla_{yy} g(x,y)$, and their variance are bounded by $\sigma_f^2, \sigma_g^2, \sigma_{g,2}^2$ and $\sigma_{g,2}^2$, respectively.

**Assumption 4.** The set $\mathcal{X}$ is nonempty. For any $x$, the set $\mathcal{Y}(x)$ is nonempty.

Assumption 1–3 are standard for stochastic bilevel optimization [8, 9, 24, 29, 32, 35, 37]. Assumption 4 is to ensure the feasibility of the problem (1). Since $A_y b = b$ has solution $y$ if and only if $AA^\dagger b = b$ according to [31], Assumption 4 is equivalent to $AA^\dagger (c - h(x)) = c - h(x)$. One sufficient but not necessary condition for Assumption 4 is that $A$ is full row rank, which does not impose any additional requirement on $h(x)$. Another sufficient but not necessary condition for Assumption 4 is $\forall x, c - h(x) \in \text{Ran}(A)$, e.g., $h = 0, c \in \text{Ran}(A)$, which does not assume $A$ is full row rank.

One of the keys to establishing $\tilde{O}(\epsilon^{-2})$ sample complexity of unconstrained bilevel optimization [8, 37] is to utilize the smoothness of $y^*(x)$. Thanks to the singular value decomposition, we can obtain the smoothness of $y^*(x)$ for linearly equality constrained LL (1b) in the following lemma, the proof of which is deferred to Appendix A.1.

**Lemma 3.** Under Assumption 1–2 and 4, $y^*(x)$ is $L_y$-Lipschitz continuous and $L_{yx}$-smooth, where the constants $L_y$ and $L_{yx}$ are specified in Appendix A.1.

However, due to the UL constraint, the proof for unconstrained stochastic bilevel optimization [8] cannot be applied even with the smoothness of $y^*(x)$ in Lemma 3. For constrained UL with LL unconstrained bilevel problem, recent works [9, 29] leveraged the Moreau envelope technique of projected SGD in [14]. However, when the stochastic gradient estimator is biased, the gradient bias term cannot be mitigated by the framework in [14]. Therefore, [29] ended up with suboptimal sample complexity $O(\epsilon^{-2.5})$, while [9] added an additional correction in the LL update. Owing to the special property of linear equality constrained UL presented in Lemma 1, we establish the $\tilde{O}(\epsilon^{-2})$ sample complexity of Algorithm 1 in the next lemma without resorting to the Moreau envelope technique. The proof is deferred to Appendix B.3.

**Theorem 1 (Convergence rate of AiPOD).** Under Assumption 1–4, if we choose

$$
\alpha = \min \left( \bar{\alpha}_1, \bar{\alpha}_2, \frac{\bar{\alpha}}{\sqrt{K}} \right), \quad \beta = \frac{5L_f L_y + L_{yx} \bar{C}_L^2}{\mu_g} \alpha, \quad N = O(\log K)
$$

where $\bar{\alpha}_1, \bar{\alpha}_2$ are defined in Appendix B.3, then for any $S = O(1)$ in Algorithm 1, we have

$$
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \| \nabla F(x^k) \|_{P_2}^2 \right] = \tilde{O} \left( \frac{1}{\sqrt{K}} \right).
$$

Theorem 1 shows that Algorithm 1 achieves $\epsilon$ stationary point by $\tilde{O}(\epsilon^{-2})$ iterations, which matches the iteration complexity of single-level projected SGD method [14]. Moreover, the sample complexity of AiPOD is $\tilde{O}(K) = \tilde{O}(\epsilon^{-2})$, which matches the unconstrained bilevel SGD method [8].
3 E-AiPOD: A Projection-efficient Variant of AiPOD

In this section, we focus on the case when evaluating projection is expensive and propose a projection efficient variant of AiPOD that we term E-AiPOD to avoid frequent projection steps.

3.1 Algorithm development

Besides the explicit projections for \( x \)- and \( y \)-updates in Algorithm 1, calculating \( w^k \) in (9b) also requires projecting \( \nabla y g(x^k, y^{k+1}; \phi_{(n)}) \) onto the null space of the LL problem, e.g., calculating \( V_2^\top \nabla y g(x^k, y^{k+1}; \phi_{(n)}) V_2 \). The explicit projections in (5) are referred as LL projections, while both the explicit projections in \( x \)-update and implicit projections contained in \( w^k \) are regarded as UL projections. We use the following ways to save projections.

Skip LL projections. We leverage a recent variant of projected SGD called Proxskip [50] in the LL update which evaluates projection lazily with probability \( 0 < p < 1 \). Fixing UL iteration \( k \) and at each LL iteration \( s \), we first perform an SGD update corrected by the residual \( r^{k,s} \) as

\[
\hat{y}^{k,s+1} = y^{k,s} - \beta (\nabla y g(x^k, y^{k,s}; \phi_{(n)}^{(k,s)}) - r^{k,s}). \tag{10a}
\]

With probability \( 1 - p \), we skip the projection and keep \( y^{k,s+1} = \hat{y}^{k,s+1}, r^{k,s+1} = r^{k,s} \); with probability \( p \), we update LL parameter \( y^{k,s} \) and the residual \( r^{k,s} \) as

\[
y^{k,s+1} = \text{Proj}_{\gamma(x^k)} (\hat{y}^{k,s+1} - \beta r^{k,s}/p) \tag{10b}
\]

\[
r^{k,s+1} = r^{k,s} + p(y^{k,s+1} - \hat{y}^{k,s+1})/\beta. \tag{10c}
\]

In (10a), \( r^{k,s} \) compensates the error of skipping projection which will be updated every \( 1/p \) rounds in expectation so that the corrected stochastic gradient update in (10a) will approximate the projected SGD update in (5). The update of residual sequences in (10b) ensures that \( r^{k,s} \) converges to the projection skipping errors at the optimal point \( y^*(x^k) \), i.e., \( \lim_{s \to \infty} r^{k,s} = \nabla y g(x^k, y^*(x^k)) =: r^*(x) \), so that the asymptotic convergence for E-AiPOD is similar to AiPOD. With \( K \) steps of UL updates and \( S \) steps of LL updates, the expected number of projection evaluations reduces from \( K \) in AiPOD to \( pKS \) in E-AiPOD. We summarize the LL update of E-AiPOD in Algorithm 3.

Use delayed \( w^k \) and reduce UL projections. At upper iteration \( k \), we calculate \( w^k \) by the Neumann series (9b) and initialize \( x^{k,0} = x^k \). Subsequently, for \( t = 0 \) to \( T - 1 \), we update \( x^{k,t+1} \) via

\[
x^{k,t+1} = x^{k,t} - \alpha h^{k,t}_f \tag{11a}
\]

where

\[
h^{k,t}_f := \nabla x f(x^{k,t}; y^{k+1}, \xi^{k,t}) + w^k. \tag{11b}
\]
We characterize its convergence rate by using a new Lyapunov function as

\[ \mathcal{V}_1^k = F(x^k) + \frac{L_f}{L_r} \left( \|y^*(x^k) - y^k\|^2 + \frac{\beta^2}{p^2} \|r^k - r^*(x^k)\|^2 \right) \]  

where \( L_f \) and \( L_r \) are constants defined in Lemma 9 and 20 in Appendix and \( r^*(x^k) = \nabla_y g(x, y^*(x)) \). The complexity bound of E-AiPOD is stated in the following theorem.

**Theorem 2 (Convergence of E-AiPOD).** Under Assumption 1–4, if we choose stepizes such that \( \alpha \delta T < \tilde{\alpha} \), where \( \tilde{\alpha} < 1 \) is a constant formally defined in (95), and let \( \beta = \mathcal{O}(\alpha T), p = \mathcal{O}(\sqrt{\beta}), S = \mathcal{O}(1), N = \mathcal{O}(\log(\alpha^{-1})) \), then the sequences generated by Algorithm 2 satisfies

\[ \frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \| \nabla F(x^k) \|_2^2 \right] \leq \frac{2(\mathcal{V}_1^0 - F^*)}{\alpha \delta T K} + 2c_1\sigma_{g,1}^2 \alpha \delta T + 2c_2\tilde{\sigma}_f^2 \alpha \delta + \mathcal{O}(\alpha^2 \delta^2 T) \]  

where \( c_1 \) and \( c_2 \) are constant formally defined in Appendix C.3, \( F^* \) is the lower bound of \( F(x) \), and \( \sigma_{g,1}^2, \tilde{\sigma}_f^2 \) are the variance of LL and UL updates.

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**Algorithm 3 E-AiPOD_{low}(x^k, y^k, r^k, \beta, p, S)**

1: Inputs: \( x^k, y^k, r^k \), stepsize \( \beta \), skipping probability \( p \), the number of LL rounds \( S \)
2: Initialization \( y^{k,0} = y^k, r^{k,0} = r^k \)
3: for \( s = 0 \) to \( S - 1 \) do
4:    update \( \tilde{y}^{k,s+1} \) by (10a)
5:    draw \( \theta^{k,s} \) with \( \mathbb{P}(\theta^{k,s} = 1) = p \)
6:    if \( \theta^{k,s} = 1 \) then
7:      update \( y^{k,s+1} \) by (10b)
8:    else
9:      \( y^{k,s+1} = \tilde{y}^{k,s+1} \)
10: end if
11: update \( r^{k,s+1} \) by (10c)
12: end for
13: Outputs: \( y^{k+1} = y^k \), \( r^{k+1} = r^k \)

---

**Algorithm 4 E2-AiPOD_{med}(x^k, y^{k+1}, \rho, q, N)**

1: Inputs: \( x^k, y^{k+1} \), stepsize \( \rho \), skipping probability \( q \), the number of rounds \( N \)
2: Initialization \( u^{k,0} = 0, e^{k,0} = 0 \)
3: for \( n = 0 \) to \( N - 1 \) do
4:    update \( u^{k,n+1} \) by (17a)
5:    draw \( \hat{\theta}^{k,n} \) with \( \mathbb{P}(\hat{\theta}^{k,n} = 1) = q \)
6:    if \( \hat{\theta}^{k,n} = 1 \) then
7:      update \( u^{k,n+1} \) by (17b)
8:    else
9:      set \( u^{k,n+1} = \tilde{u}^{k,n+1} \)
10: end if
11: update \( e^{k,n+1} \) by (17c)
12: end for
13: Outputs: \( u^{k+1} = u^k \)
With proper choices of $\alpha$ and $\delta$, the four terms in (14) could vanish simultaneously. The following corollary shows the results for vanilla periodical projections when $\delta = 1$.

**Corollary 1 (Reduction of LL projection).** Under the same condition of Theorem 2, if we choose $\alpha = \frac{\bar{\alpha}}{TK\sqrt{K}}$, $\delta = 1$, the convergence rate of Algorithm 2 is

$$
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \|\nabla F(x^k)\|_2^2 \right] = \tilde{O} \left( \frac{1}{\sqrt{K}} \right).
$$

Since $K = \tilde{O}(\epsilon^{-2})$ and $p = O(\sqrt{\beta}) = O(K^{-\frac{1}{2}})$, the total number of LL projections reduces to

$$pKS = O(K^{\frac{3}{2}}) = \tilde{O}(\epsilon^{-1.5}).$$

Corollary 1 implies that the convergence rate of E-AiPOD is the same as that of AiPOD when $\delta = 1$, but the LL projection complexity can be reduced to $\tilde{O}(\epsilon^{-1.5})$. Compared with Proxskip [50] which improves the projection complexity on $\kappa = \ell_g, 1/\mu_g$, we can further achieve the reduction on $\epsilon$ owing to the smaller LL stepsize $\beta = O(1/\sqrt{K})$. Besides, the next corollary shows the benefit for enlarging $\delta$, which further reduces the iteration and projection complexity of E-AiPOD.

**Corollary 2 (Reduction of UL projection).** Under the same condition of Theorem 2, if we choose $\alpha = \frac{\bar{\alpha}}{TK\sqrt{K}}$, $\delta = \sqrt{T}$ with $T < K$, and select LL batch size as $O(T)$ such that $\sigma_g^2 = O(1/T)$, then the convergence rate of Algorithm 2 is

$$
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \|\nabla F(x^k)\|_2^2 \right] = \tilde{O} \left( \frac{1}{\sqrt{TK}} \right).
$$

As a result, the sample complexity of E-AiPOD for both UL and LL are $\tilde{O}(TK) = \tilde{O}(\epsilon^{-2})$, while the total number of the UL and LL projection are respectively, reduced to

$$UL : K + KN = \tilde{O}(\epsilon^{-2}/T), \quad \text{and} \quad LL : pKS = O(K^{\frac{3}{2}}) = \tilde{O}(\epsilon^{-1.5}/T^{\frac{1}{2}}).$$

Corollary 2 implies with larger $\delta$, increasing $T$ can accelerate the convergence rate and improve the projection complexity without degrading the sample complexity for both levels. Compared with the single-level case, $\sigma_g^2$ can be seen as the additional error caused by the LL stochasticity. The idea behind reducing the UL projection complexity is to reduce the variance of the averaged gradient estimator by $T$ gradient descent steps and use larger $\delta$ to balance the projection frequency. However, this can not reduce the variance of LL; see the different terms for $\tilde{\sigma}_g^2$ and $\sigma_g^2$ over $T$ in (14). Therefore, we need to increase the LL batch size correspondingly to reduce $\sigma_g^2$ in the bilevel problem. By virtue of the faster rate, the sample complexity for LL is $\tilde{O}(K)$, which is still $\tilde{O}(\epsilon^{-2})$.

### 4 E2-AiPOD: A Projection-efficient Variant of AiPOD without Coupling Constraints

In Section 3, we have developed E-AiPOD that reduces both UL and LL projection complexity with an increasing LL batch size $O(T)$. The essential obstacle for preventing E-AiPOD from using constant LL batch size is that the delayed $w^k$ in (11b) would bring error to the UL gradient estimator. This section overcomes this obstacle in the setting where the LL constraints are independent of UL variable $x$, i.e., $h(x) = 0$, and introduces E2-AiPOD - another projection-efficient variant of AiPOD that reduces both UL and LL projection complexity with a constant LL batch size.
4.1 Algorithm development

**Intuition.** We first provide some intuition of the proposed E2-AiPOD method via the deterministic version of (1). Instead of calculating \( w^k \) in (9b) of E-AiPOD which requires expected projections \( N \) times, we can approximate \( w^k \) by a sequence and then use the idea of skipping projections to reduce the number of projections. According to (6) and (8) and letting \( h(x) = 0 \), it follows that the UL gradient of (1) can also be given by

\[
\nabla F(x) = \nabla_x f(x, y^*(x)) + \nabla_{xy} g(x, y^*(x)) u^*(x, y^*(x))
\]

where \( u^*(x, y) := -V_2 \left( V_2^T \nabla_{yy} g(x, y) V_2 \right)^{-1} V_2^T \nabla_y f(x, y). \) (15)

In E-AiPOD, \( u^*(x^k, y^{k+1}) \) is estimated via Neumann series to approximate the Hessian inverse; see (9a). Instead, we can view \( u^*(x, y) \) as an optimal solution of a linear constrained quadratic programming and approximate it using iterative methods. Formally, we have the following lemma.

**Lemma 4 (Equivalent characterization of \( u^*(x, y) \)).** The Hessian inverse estimator \( u^*(x, y) \) is the minimizer of a \( \mu_y \)-strongly convex function over a linear space, that is

\[
u^*(x, y) = \arg \min_{u \in \{u| V_1^T u = 0\}} \frac{1}{2} \left\| \nabla_{yy}^2 g(x, y) \nabla_y f(x, y) + \nabla_{yy}^2 g(x, y) u \right\|^2.
\]

where \( V_1 \) is the orthogonal basis of \( \text{Ran}(A^\top) \).

Thanks to the above lemma, we can treat \( u^*(x^k, y^{k+1}) \) as an optimal solution of an optimization problem and iteratively update another sequence \( \{u^{k,n}\} \) to approximate it. As a consequence, the solution of the original problem (1) can be obtained by three coupled sequences. For simplicity, we call the optimization with respect to \( u^*(x, y) \) the medium-level (ML) problem. Assuming that \( \{\phi^k, \phi^{k,0}, \ldots, \phi^{k,S-1}, \ldots, \phi^{k}_{(0)}, \ldots, \phi^{k}_{(N-1)}\} \) and \( \{\xi^k, \xi^k_{(0)}, \ldots, \xi^k_{(N-1)}\} \) are i.i.d samples, we then elaborate the procedure of E2-AiPOD.

**Skip LL projections.** The LL update for E2-AiPOD is identical to E-AiPOD.

**Skip UL implicit projections.** The implicit UL projections correspond to the ML projections. We update \( u^k \) by \( N \)-step lazily projected SGD with corrections, which is in the same spirit of the LL \( y \)-update. Specifically, for any UL iteration \( k \), we first initialize \( u^{k,0} = e^{k,0} = 0 \). For a given ML iteration \( n \), instead of using a projected SGD iteration, we update \( u^{k,n+1} \) via the SGD iteration for (16) corrected by \( e^{k,n} \) that compensates the projection error, that is

\[
\hat{u}^{k,n+1} = u^{k,n} - \rho \left( \nabla_y f(x^k, y^{k+1}; \xi_{(n)}) + \nabla_{yy} g(x^k, y^{k+1}; \phi_{(n)}) u^{k,n} - e^{k,n} \right)
\]

**Algorithm 5** E2-AiPOD for constrained bilevel problem

1: Initialization: \( x^0, y^0 \), stepsizes \( \{\alpha, \beta, \rho\} \), the number of rounds \( \{S, N, K\} \) and projection frequency \( \{p, q, T\} \).
2: for \( k = 0 \) to \( K - 1 \) do
3: \( \{y^{k+1}, r^{k+1}\} = E\text{-AiPOD}_{\text{low}}(x^k, y^k, r^k, \beta, p, S) \)
4: update \( u^{k+1} = E\text{-AiPOD}_{\text{med}}(x^k, y^{k+1}, \rho, q, N) \)
5: compute \( d^k_f \) defined in (18a).
6: if \( k \mod T = 0 \) then
7: update \( x^{k+1} = \text{Proj}_\mathcal{X}(x^k - \alpha d^k_f) \) in (18b)
8: else
9: update \( x^{k+1} = x^k - \alpha d^k_f \)
10: end if
11: end for
where \( \rho > 0 \) is the stepsize of the ML update. Subsequently, with probability \( 1 - q \), we keep \( u^{k,n+1} = \hat{u}^{k,n+1}, e^{k,n+1} = e^{k,n+1} \); with probability \( q \), we update \( u^{k,n+1} \) and the \( e^{k,n+1} \) as

\[
\begin{align*}
u^{k,n+1} &= V_2 V_2^T \left( \hat{u}^{k,n+1} - \rho e^{k,n}/q \right) \\
e^{k,n+1} &= e^{k,n} + q(\hat{u}^{k,n+1} - \hat{u}^{k,n+1})/\rho.
\end{align*}
\] (17b) (17c)

After \( N \) rounds, we set \( u^{k+1} = u^{k,N} \) and \( e^{k+1} = e^{k,N} \).

**Lazy UL explicit projections.** Similar to E-AiPOD, we perform the UL projection every \( T \geq 1 \) rounds but we formulate it in a different scheme. Specifically, if \( k \mod T = 0 \), we perform the projected SGD in (18b); otherwise, we update \( x^{k+1} \) by SGD via \( \ell_f^k \) defined in (18a).

\[
\begin{align*}
\ell_f^k &:= \nabla_x f(x^k, y^{k+1}; \xi^k) + \nabla_y g(x^k, y^{k+1}; \phi^k) u^{k+1} 
\end{align*}
\] (18a)

\[
\begin{align*}
x^{k+1} &= \text{Proj}_{x^\mathcal{A}}(x^k - \alpha \ell_f^k)
\end{align*}
\] (18b)

The benefits of viewing the projected SGD in this way other than describing it by another loop as in E-AiPOD are that: 1) the total number of UL projections is \( \mathcal{O}(K/T) \) rather than \( \mathcal{O}(K) \); and, 2) it is more convenient to incorporate the ML sequences of E2-AiPOD in this UL framework to obtain the improved projection complexity, which will be elaborated more in detail in Section 4.2.

We summarize the E2-AiPOD algorithm in Algorithm 5 that encompasses E-AiPOD \(_{low}\) and E2-AiPOD \(_{mod}\) as subroutines.

### 4.2 Theoretical analysis

The recent advances in stochastic approximation with multiple coupled sequences have revealed that one of the keys to establishing the \( \tilde{\mathcal{O}}(\epsilon^{-2}) \) overall sample complexity for multi-sequences is the Lipschitz smoothness of the fixed point [53]. However, this property does not hold for \( u^*(x, y) \) unless one makes extra assumption that \( \nabla_{yy} g(x, y) \) and \( \nabla_{yx} g(x, y) \) are Lipschitz continuous like in [13]. Alternatively, we establish \( \tilde{\mathcal{O}}(\epsilon^{-2}) \) sample complexity for E2-AiPOD by the virtue of boundedness of \( u^*(x, y) \), which is established in Lemma 22.

To characterize the convergence of E2-AiPOD, we use another Lyapunov function defined as

\[
\mathcal{V}_2^k := F(\tilde{x}^k) + \frac{L_f}{L_r} \left( \|y^k - y^*(\tilde{x}^k)\|^2 + \frac{\beta^2}{p^2} \|r^k - r^*(\tilde{x}^k)\|^2 \right)
\] (19)

where \( \tilde{x}^k = \text{Proj}_{x^\mathcal{A}}(x^k) \) is a virtual sequence and \( L_f, L_r \) are defined in Lemma 9 and 20 in Appendix.

We also treat the UL \( x \)-update of E2-AiPOD as the biased SGD, but the reference point of \( x^k \) has been changed to the virtual point \( \tilde{x}^k \) rather than the most-recent projection point \( x^k \) in E-AiPOD with \( k \mod T = 0 \). The reasons lie in three folds: 1) \( \tilde{x}^k \) can be served as a reference point as we can prove that it is close to \( x^k \) in the sense \( \mathbb{E}[\|x^k - \tilde{x}^k\|^2] = \mathcal{O}(\alpha^2) \); 2) the virtual point \( \tilde{x}^k \) can measure error due to the one-step projection-free deviation at \( x^k \); and, 3) the corrections at ML compensate the one-step projection-free errors so that the convergence is provable by using the reference point \( \tilde{x}^k \).

The convergence of E2-AiPOD is stated in Theorem 3 with its proof deferred in Appendix D.5.

**Theorem 3 (Convergence of E2-AiPOD).** Under Assumption 1–4, if we choose stepsizes such that

\[
\beta = \mathcal{O}(\alpha), \beta \leq \frac{1}{L_{g,1}} \text{ and } \rho \leq \min \left\{ \frac{1}{L_{g,1}}, \frac{\mu_g}{4\sigma_{g,2}^2} \right\}, \text{ the probabilities } p = \mathcal{O}(\sqrt{\beta}), q = \mathcal{O}(\sqrt{\rho}) \text{ and the}
\]
number of ML and LL steps \( N = O(\log(\alpha^{-1})) \), \( S = O(1) \), then the sequences of Algorithm 5 satisfy
\[
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \| \nabla F(\tilde{x}^k) \|^2_{\mathcal{P}_x} \right] \leq \frac{2(\mathcal{V}_0 - F^*)}{\alpha K} + O(\alpha \sigma_{g,1}^2 + \alpha^2 T^2 + \alpha \tilde{\sigma}_{f,2}^2 + \rho \sigma_u^2) \tag{20}
\]
where \( \tilde{x}^k = \text{Proj}_y x^k \), \( P_x = I - B^\top B \), \( F^* \) is the lower bound of \( F(x) \) and \( \sigma_{g,1}^2, \sigma_u^2, \tilde{\sigma}_{f,2}^2 \) are the variance of LL, ML, and UL updates.

We can choose \( T, \alpha \) and \( \rho \) to balance the right hand side of (20), which leads to the following corollary.

**Corollary 3 (Sample and projection complexity of E2-AiPOD).** Under Assumption 1–4, if we choose stepsizes \( \alpha = O(1/\sqrt{K}) \), \( \rho = \beta = O(1/\sqrt{K}) \), probabilities \( p = O(K^{-1/4}) \), \( q = O(K^{-1/4}) \), \( T = O(K^{1/4}) \) and the number of steps \( N = O(\log(K)) \), \( S = O(1) \), the sequences of E2-AiPOD satisfy
\[
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \| \nabla F(\tilde{x}^k) \|^2_{\mathcal{P}_x} \right] = O\left( \frac{1}{\sqrt{K}} \right).
\]
As a result, the sample complexity of Algorithm 5 is \( KNS = \tilde{O}(\epsilon^{-2}) \), and the expected number of projections of UL and LL are respectively

UL projections: \( K/T + qKN = \tilde{O}(K^{3/4}) = \tilde{O}(\epsilon^{-1.5}) \), LL projections: \( pKS = O(K^{5/4}) = O(\epsilon^{-1.5}) \).

Compared with E-AiPOD, E2-AiPOD can reduce the UL projection complexity with respect to \( \epsilon \) with constant \( O(1) \) LL batch size owing to the corrections in Hessian skipping stages, which makes it more compatible for large-scale bilevel problems.

### 5 Applications to Federated Bilevel Learning

Consider the bilevel federated learning problem \([57]\) in the following form
\[
\min_{x \in \mathcal{X}} F(x) = \frac{1}{M} \sum_{m=1}^{M} f_m(x_m, y_m(x_m)) \quad \text{s.t.} \quad y^*(x) = \arg\min_{y \in \mathcal{Y}} \frac{1}{M} \sum_{m=1}^{M} g_m(x_m, y_m) \tag{21}
\]
where each client \( m \in [M] := \{1, \cdots, M\} \) maintains its local model \( x_m, y_m \) and is only accessible to its individual function \( (f_m, g_m) \). Let \( x = [x_1, \cdots, x_M]^{\top} \) and \( y = [y_1, \cdots, y_M]^{\top} \) denote the collection of individual models; \( y^*(x) = [y_1^*(x_1), \cdots, y_M^*((x_M))]^{\top} \) is the optimal LL model; and let \( \mathcal{X} = \{x \mid x_1 = \cdots = x_M\} \) and \( \mathcal{Y} = \{y \mid y_1 = \cdots = y_M\} \) denote the consensus set.

With \( I_d \in \mathbb{R}^{d \times d} \) denoting as the identity matrix and \( I_M \in \mathbb{R}^{M} \) denoting as the all-1 vector, we can define the consensus matrix \( A \) and calculate the orthogonal basis of its kernel as
\[
A := \begin{bmatrix}
1 & -1 \\
\vdots & \ddots \\
1 & -1
\end{bmatrix} \otimes I_d, \quad \text{and} \quad V_2 := \frac{I_M}{\sqrt{M}} \otimes I_d \tag{22}
\]
where \( \otimes \) is the Kronecker product, \( A \in \mathbb{R}^{d(M-1) \times dM} \) and \( V_2 \in \mathbb{R}^{dM \times d} \). We can define \( B \) the same as \( A \). In the federated bilevel learning setting, with \( e = c = h(x) = 0 \), the UL and LL constraint sets become \( \mathcal{X} = \{x \mid Bx = 0\} \) and \( \mathcal{Y} = \{y \mid Ay = 0\} \).
Table 2: Communication comparison of E-AiPOD, E2-AiPOD and the state-of-the-art works FedNest in [57] on stochastic federated bilevel learning to achieve $\epsilon$ stationary point.

| Method       | UL communication | LL communication |
|--------------|------------------|------------------|
| E-AiPOD      | $\tilde{O}(\epsilon^{-2}/T)$ | $\tilde{O}(\epsilon^{-1.5})$ |
| E2-AiPOD     | $\tilde{O}(\epsilon^{-1.5}/T^{\frac{1}{2}})$ | $\tilde{O}(\epsilon^{-2})$ |
| FedNest      | $\tilde{O}(\epsilon^{-1.5})$ | $\tilde{O}(\epsilon^{-2})$ |

Therefore, in the federated bilevel setting (21), the UL gradient in (6) can be specialized as

$$\nabla F(x) = [\nabla_{x_1} F(x), \ldots, \nabla_{x_M} F(x)]^T,$$

where each block $\nabla_{x_m} F(x)$ is defined as

$$\nabla_{x_m} F(x) = \nabla_{x_m} f_m(x_m, y_m^*(x_m)) + \frac{\nabla y_m^T(x_m)}{M} \sum_{m=1}^M \nabla y_m f_m(x_m, y_m^*(x_m)) \tag{23a}$$

with

$$\nabla y_m^*(x_m) = - \left( \frac{1}{M} \sum_{m=1}^M \nabla y g_m(x_m, y_m^*(x_m)) \right)^{-1} \nabla y x g_m(x_m, y_m^*(x_m)). \tag{23b}$$

Besides, from (22), the projections amount to averaging $x_m$ and $y_m$, i.e.,

$$\text{Proj}_{x|Bx=0}(x) = (\bar{x}, \ldots, \bar{x}), \quad \text{with} \quad \bar{x} = \frac{1}{M} \sum_{m=1}^M x_m \tag{24a}$$

$$\text{Proj}_{y|Ay=0}(y) = (\bar{y}, \ldots, \bar{y}), \quad \text{with} \quad \bar{y} = \frac{1}{M} \sum_{m=1}^M y_m. \tag{24b}$$

Therefore, in the federated bilevel learning setting, the UL and LL projections in E-AiPOD and E2-AiPOD correspond to communicating the UL and LL variables between clients and the server. With the above facts, we are able to apply E-AiPOD and E2-AiPOD to the federated bilevel setting, which are summarized in Algorithm 6 together in Appendix.

5.1 Communication complexity in federated bilevel optimization

The weighted norm measure (4) in our analysis coincides with the optimality measure in the federated bilevel learning [57]; see the proof in Appendix E.2. Moreover, since Assumption 4 directly holds in federated bilevel setting, our theoretical results are based on the standard assumptions in unconstrained bilevel optimization [8, 24, 29, 32]. Inheriting from the projection complexity of E-AiPOD and E2-AiPOD, their communication complexity is stated in the next corollary.

**Corollary 4 (Communication complexity).** Under Assumption 1–3 and the same condition of Corollary 2, the total number of the UL communication of Algorithm 6 with option E-AiPOD is reduced to $\tilde{O}(\epsilon^{-2}/T)$, while the LL communication is reduced to $\tilde{O}(\epsilon^{-1.5}/T^{\frac{1}{2}})$. Under the same condition of Corollary 3, the total number of the UL communication of Algorithm 6 with option E2-AiPOD is reduced to $\tilde{O}(\epsilon^{-1.5})$, while the LL communication is reduced to $\tilde{O}(\epsilon^{-1.5})$. 

---

| Method       | UL communication | LL communication |
|--------------|------------------|------------------|
| E-AiPOD      | $\tilde{O}(\epsilon^{-2}/T)$ | $\tilde{O}(\epsilon^{-1.5})$ |
| E2-AiPOD     | $\tilde{O}(\epsilon^{-1.5}/T^{\frac{1}{2}})$ | $\tilde{O}(\epsilon^{-2})$ |
| FedNest      | $\tilde{O}(\epsilon^{-1.5})$ | $\tilde{O}(\epsilon^{-2})$ |
Compared with the state-of-the-art work FedNest [57], the communication complexity of E-AiPOD and E2-AiPOD for federated learning in Algorithm 6 reduces from $\tilde{O}(\epsilon^{-2})$ to $\tilde{O}(\epsilon^{-1.5})$ even if we use SGD-type updates instead of SVRG-type in FedNest. See a detailed summary in Table 2.

5.2 Additional related works on bilevel federated learning

There is a rich literature in federated learning and recently bilevel federated learning. Federated learning and the Federated average (FedAvg) algorithm were first introduced by [49]. The convergence rate of FedAvg has been thoroughly investigated by [55, 60, 61, 66]; see a survey [34]. Later on, [51] applied variance reduction techniques to tackle the heterogeneous data and obtain the linear convergence for strongly convex objectives. Recently, [50] has first theoretically achieved the optimal complexity for strongly convex objectives without assuming any data similarity.

The federated bilevel learning has been first studied in [57] that aims to tackle federated learning problems to with the nested structure. The FedNest algorithm has been developed in [57] that achieves both $\tilde{O}(\epsilon^{-2})$ sample and communication complexity. The complexity of FedNest has been improved to $\tilde{O}(\epsilon^{-1.5})$ by using momentum-based variance-reduction technique in LocalBSGVRM [21] and FedBiOAcc [38], but these two works consider different settings than FedNest and our paper. Specifically, FedBiOAcc [38] only considered the UL federated setting. More importantly, the additional bounded data similarity assumption is enforced in [21, 38] that allows to bypass the key challenge of estimating the global Hessian. From the algorithmic perspective, LocalBSGVRM and FedBiOAcc achieve the improved communication complexity partially thanks to the accelerated $\tilde{O}(\epsilon^{-1.5})$ iteration complexity of the non-federated momentum-based bilevel algorithms [35, 62], while E-AiPOD and E2-AiPOD are based on SGD-based bilevel algorithms [8, 32] with $\tilde{O}(\epsilon^{-2})$ iteration complexity. Therefore, it would be interesting to see in future work if incorporating momentum acceleration in E-AiPOD and E2-AiPOD can further reduce communication complexity.

Recent advances in this line have also considered different settings such as decentralized, deterministic or finite-sum settings; see e.g., [10, 22, 30, 44, 45, 63]. While it is not the focus here, it is also promising to extend E2-AiPOD to the decentralized bilevel setting with the same projection (communication) complexity guarantee by leveraging the decentralized version of Proxskip in [50] to the LL and ML, and replacing the periodical SGD with decentralized SGD in the UL level.

6 Experiments

To validate the theoretical results and evaluate the empirical performance of our proposed methods, this section conducts experiments in both synthetic tests and federated bilevel learning tasks including representation learning and learning from imbalanced data.

6.1 Synthetic experiments

We first consider a special case of the equality-constrained bilevel problem (1), given by

$$\min_{x \in X} F(x) = \sin (c^\top x + d^\top y^*(x)) + \ln \left(\|x + y^*(x)\|^2 + 1\right), \text{ s.t. } y^*(x) = \arg\min_{y \in \mathcal{Y}(x)} \frac{1}{2}\|x - y\|^2$$

where $X = \{x \mid Bx = 0\} \subset \mathbb{R}^{100}$, $\mathcal{Y}(x) = \{y \mid Ay + Hx = 0\} \subset \mathbb{R}^{100}$, and $A, B, H, c, d$ are randomly generated non-zero matrices or vectors that satisfy Assumption 4. To guarantee that $\mathcal{Y}(x)$...
and $\mathcal{X}$ are not singleton, the matrices $A$ and $B$ are rank-deficient matrices. In the simulation, we use the noisy versions of the gradients where a Gaussian noise with zero mean and a standard deviation of 0.1 is added. It can then be checked that in this setting, Assumptions 1–4 are satisfied.

The test results are reported in Figure 1. In the left figure, we test the impact of the probability $p$ on the projection complexity and the iteration complexity. It can be observed that E-AiPOD with relatively small $p$ has almost the same iteration complexity (as indicated in the lower left figure) while it significantly saves projection rounds (see upper left figure). We also compare AiPOD and E-AiPOD in the right figure. It can be observed that E-AiPOD is able to save projection while maintaining the same iteration complexity as that of AiPOD, which is consistent with our theoretical result.

6.2 Federated representation learning

In this section, we apply E-AiPOD in Algorithm 6 to the federated representation learning task. The classic machine learning approach learns a data representation and a downstream header jointly on the training data set. While the bilevel representation learning [20] seeks to learn a data representation on the validation set and a header on the training data set, the procedure can then be formulated as a bilevel problem. In a federated representation learning setting with $M = 50$ clients, the validation and training data sets are distributed among clients, and the goal is to learn a representation and header respectively on the joint validation and training data set while protecting data privacy.

Formally, the problem can be formulated as an instance of (21), given by

$$
\min_{x \in \mathcal{X}} \frac{1}{M} \sum_{m=1}^{M} f_{ce}(x_m, y^*_m(x); D^{m}_{\text{val}}), \quad \text{s.t.} \quad y^*(x) = \arg\min_{y \in \mathcal{Y}} \frac{1}{M} \sum_{m=1}^{M} f_{ce}(x, y_m; D^{m}_{\text{tr}}) + 0.05\|y_m\|^2,
$$

where $x$ is the parameters of the representation layer; $y$ is the parameter of the classifier layer; $D^{m}_{\text{tr}}$ and $D^{m}_{\text{val}}$ are, respectively, the training and validation set of client $m$; $\mathcal{X}$ and $\mathcal{Y}$ are the consensus sets.
defined in (21). The cross-entropy loss $f_{ce}$ is defined as

\[
f_{ce}(x, y; D) := - \frac{1}{|D|} \sum_{d_n \in D} \log \frac{\exp (h_n(x, y; d_n))}{\sum_{c=1}^{C} \exp (h_c(x, y; d_n))}
\]

where $C$ is the number of classes, $d_n$ is the $n$-th data from class $l_n$ in data set $D$ and $h(x, y; d_n) = [h_1(x, y; d_n), ..., h_C(x, y; d_n)]^\top \in \mathbb{R}^C$ is the output of the model with parameter $(x, y)$ and input $d_n$.

The experimental results are reported in Figure 2. From the left figure of Figure 2, a relatively small value of $p$ helps save communication rounds while a too small value of $p$ might degrade performance. With a properly chosen $p = 0.1$, it can be observed from the right figure that E-AiPOD outperforms FedNest [57] in terms of communication complexity.

### 6.3 Federated learning from imbalanced data

In this subsection, we apply E-AiPOD to the federated learning from the imbalanced data task, where the goal is to learn a good model that guarantees both fairness and generalization from datasets with under-represented classes [39]. In the UL, the loss-tuning parameters are trained to improve generalization and fairness, while the model parameters are trained on a possibly imbalanced data-set.
in the LL. The method was later extended to the federated setting in [57]. Formally, the problem can be written as a case of (21), given by

$$\min_{x \in \mathcal{X}} \frac{1}{M} \sum_{m=1}^{M} f_{\text{up}}^{m}(x, y_{m}^{*}(x); \mathcal{D}_{\text{val}}^{m}), \quad \text{s.t.} \quad y^{*}(x) = \arg \min_{y \in \mathcal{Y}} \frac{1}{M} \sum_{m=1}^{M} f_{\text{low}}^{m}(x, y_{m}; \mathcal{D}_{\text{tr}}^{m}),$$

where the number of clients is $M = 50$, $x$ is the loss-tuning parameters and $y$ is the neural network parameter. Here $\mathcal{D}_{\text{tr}}^{m}$ and $\mathcal{D}_{\text{val}}^{m}$ are respectively the training and validation set of client $m$ and $\mathcal{X}$, $\mathcal{Y}$ are the consensus sets defined in (21). From [36], the so-called vector-scaling loss $f_{\text{low}}^{m}$ is defined as

$$f_{\text{low}}^{m}(x, y; \mathcal{D}) := -\frac{1}{|\mathcal{D}|} \sum_{d_{n} \in \mathcal{D}} \omega_{l_{n}} \log \frac{\exp (\delta_{l_{n}} h_{l_{n}}(y; d_{n}) + \tau_{l_{n}})}{\sum_{c=1}^{C} \exp (\delta_{c} h_{c}(y; d_{n}) + \tau_{c})}$$

where $N$ is the data set size, $C$ is the number of classes, $d_{n}$ is the $n$-th data with label class $l_{n}$ in data set $\mathcal{D}$ and $h(y; d_{n}) = [h_{1}(y; d_{n}), ..., h_{C}(y; d_{n})]^{\top} \in \mathbb{R}^{C}$ is the logit output of the neural network with parameter $y$ and input $d_{n}$. Define $x = (\omega, \delta, \tau)$ where $\omega := [\omega_{1}, ..., \omega_{C}]^{\top} \in \mathbb{R}^{C}$ and $\delta, \tau$ can be defined similarly. The upper-level loss $f_{\text{up}}^{m}$ is a special case of $f_{\text{low}}^{m}$ with $\delta = 1$ and $\tau = 0$.

The experimental results are reported in Figure 3. From the left figure of Figure 3, a relatively small value of $p$ helps save communication rounds. With $p = 0.3$, it can be observed from the right figure that E-AiPOD outperforms FedNest in terms of communication complexity. A larger $T$ results in faster convergence at the start, but is ultimately equaled by $T = 1$.

7 Conclusions

In this paper, we established the first finite-time convergence of alternating implicit projected SGD algorithm (AiPOD) for equality-constrained bilevel problems which matches the state-of-the-art result in unconstrained bilevel setting and also its single-level projected SGD. Besides, we propose two projection-efficient variants E-AiPOD and E2-AiPOD for the setting where evaluating projection is costly. E-AiPOD enjoys the $\tilde{O}(\epsilon^{-2}/T)$ upper-level and $\tilde{O}(\epsilon^{-1.5}/T^{2})$ lower-level projection complexity with $O(T)$ lower-level batch size, and E2-AiPOD enjoys $\tilde{O}(\epsilon^{-1.5})$ upper-level and lower-level projection complexity with $O(1)$ batch size. We apply E-AiPOD and E2-AiPOD on federated bilevel settings and achieve the reduction of communication complexity over the state-of-the-art work. Extensive experiments on numerical examples, federated representative learning, and federated learning from imbalanced data verify our theoretical results and demonstrate the effectiveness of our methods.

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Appendix for “Alternating Implicit Projected SGD and Its Efficient Variants for Equality-constrained Bilevel Optimization”

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A Preliminaries

A.1 Proof of Lemmas 1–3

Definition 1. Suppose $\mathcal{L} : \mathbb{R}^{d_1} \rightarrow \mathbb{R}^{d_2}$ such that each of its first-order partial derivatives exist on $\mathbb{R}^d$, then its Jacobian is defined as

$$
\nabla \mathcal{L} = \begin{bmatrix}
\frac{\partial \mathcal{L}_1}{\partial x_1} & \ldots & \frac{\partial \mathcal{L}_1}{\partial x_{d_1}} \\
\vdots & \ddots & \vdots \\
\frac{\partial \mathcal{L}_{d_2}}{\partial x_1} & \ldots & \frac{\partial \mathcal{L}_{d_2}}{\partial x_{d_1}}
\end{bmatrix}.
$$

(25)
Therefore, \( \nabla h(x) \) and \( \nabla y^*(x) \) can be written as

\[
\nabla h(x) = \begin{bmatrix}
\frac{\partial h_1}{\partial x_1} & \cdots & \frac{\partial h_1}{\partial x_d} \\
\vdots & \ddots & \vdots \\
\frac{\partial h_m}{\partial x_1} & \cdots & \frac{\partial h_m}{\partial x_d}
\end{bmatrix}, \quad \nabla y^*(x) = \begin{bmatrix}
\frac{\partial y^*_1(x)}{\partial x_1} & \cdots & \frac{\partial y^*_1(x)}{\partial x_d} \\
\vdots & \ddots & \vdots \\
\frac{\partial y^*_m(x)}{\partial x_1} & \cdots & \frac{\partial y^*_m(x)}{\partial x_d}
\end{bmatrix}.
\]

(26)

**Definition 2.** The Bregman divergence of a differentiable function \( \mathcal{L} : \mathbb{R}^d \to \mathbb{R} \) is defined as

\[
D_{\mathcal{L}}(u, v) := \mathcal{L}(u) - \mathcal{L}(v) - \langle \nabla \mathcal{L}(v), u - v \rangle.
\]

For an \( L \)-smooth and \( \mu \)-strongly convex function \( \mathcal{L} \), we have

\[
\frac{\mu}{2} \|u - v\|^2 \leq D_{\mathcal{L}}(u, v) \leq \frac{L}{2} \|u - v\|^2
\]

and

\[
\frac{1}{2L} \|\nabla \mathcal{L}(u) - \nabla \mathcal{L}(v)\|^2 \leq D_{\mathcal{L}}(u, v) \leq \frac{1}{2\mu} \|\nabla \mathcal{L}(u) - \nabla \mathcal{L}(v)\|^2.
\]

(27) \hspace{1cm} (28)

Moreover, for any \( u, v \), we have \( \langle \nabla \mathcal{L}(u) - \nabla \mathcal{L}(v), u - v \rangle = D_{\mathcal{L}}(u, v) + D_{\mathcal{L}}(v, u) \).

**Lemma 5 ([15, Proposition 4.3]).** Consider random matrices \( X \) and \( Y \) of the same size that satisfies \( \mathbb{E}[Y|X] = 0 \), then it holds \( \mathbb{E}[\|X + Y\|^2] \leq \mathbb{E}[\|X\|^2] + \mathbb{E}[\|Y\|^2] \).

**Lemma 6 (Closed form linear operator of projection).** For any nonempty linear space \( C = \{ z \mid Az + b = 0 \} \), the projection operator has the following closed form

\[
\text{Proj}_C(x) = (I - A^\dagger A)x - A^\dagger b
\]

(29)

where \( A^\dagger \) is the Moore-Penrose inverse of \( A \).

**Proof:** **Case 1.** We first consider the case where \( b = 0 \).

We denote \( P = I - A^\dagger A \), then \( C = \text{Ker}(A) \). According to Proposition 3.3. in [2], we know that \( P \) is an orthogonal projection and

\[
C = \text{Ker}(A) = \text{Ran}(P), \quad C^\perp = \text{Ker}(A)^\perp = \text{Ran}(A^\dagger) \supset \text{Ran}(A^\dagger A) = \text{Ran}(I - P)
\]

where (a) holds since \( A^\dagger = A^\dagger A A^\dagger \) [2] and

\[
\forall z = A^\dagger Aw, z = A^\dagger(Aw) \Rightarrow \text{Ran}(A^\dagger A) \subset \text{Ran}(A^\dagger),
\]

\[
\forall z = A^\dagger w, z = A^\dagger A(A^\dagger w) \Rightarrow \text{Ran}(A^\dagger) \subset \text{Ran}(A^\dagger A).
\]

Thus, for any \( x \), we can write \( x = Px + (I - P)x \) and \( Px \perp (I - P)x \), which means \( Px \) is the orthogonal projection. Then due to the uniqueness of the orthogonal decomposition, \( \text{Proj}_C(x) = Px \).

**Case 2.** We then consider the case when \( b \neq 0 \).

For any \( z \in C \), we have \( z + A^\dagger b \in \text{Ker}(A) \) since

\[
A(z + A^\dagger b) = Az + AA^\dagger b = -b + AA^\dagger b \overset{(a)}{=} 0
\]
where (a) holds since $C$ is nonempty if and only if $AA^\dagger b = b$ [31]. Similarly, we can prove for any $z \in \text{Ker}(A)$, $z - A^\dagger b \in C$. Thus, $\text{Ker}(A) = C + A^\dagger b$.

Moreover, since projection operator minimizes the distance to set $C$, we have

$$\text{Proj}_C(x) = \arg \min_{z \in C} \|z - x\|^2 = \arg \min_{z \in C} \|z + A^\dagger b - (x + A^\dagger b)\|^2$$

\begin{align*}
&\equiv a \left\{ \arg \min_{w \in \text{Ker}(A)} \|w - (x + A^\dagger b)\|^2 \right\} - A^\dagger b \\
&= \text{Proj}_{\text{Ker}(A)}(x + A^\dagger b) - A^\dagger b \\
&\equiv b P(x + A^\dagger b) - A^\dagger b \\
&\equiv c (I - A^\dagger A)x - A^\dagger b
\end{align*}

where (a) is due to $\text{Ker}(A) = C + A^\dagger b$, (b) comes from Case 1, and (c) is derived from the definition of $P$ and $(I - A^\dagger A)A^\dagger b = (A^\dagger - A^\dagger AA^\dagger) b = 0$.

By using the special property of projection on linear space, we prove Lemma 1 next.

**Restatement of Lemma 1 (Stationarity measure under linear equality constraints).** For any $x \in \mathcal{X}$ and any $\lambda > 0$, it holds that

$$\|\nabla F(x)\|_{P_x}^2 = \|\lambda^{-1}(x - \text{Proj}_{\mathcal{X}}(x - \lambda\nabla F(x)))\|^2$$

where $P_x = I - B^\dagger B$.

**Proof:** For any $\lambda$, according to (29), we have

$$\lambda^{-1}(x - \text{Proj}_{\mathcal{X}}(x - \lambda\nabla F(x))) = \lambda^{-1}(x - (I - B^\dagger B)(x - \lambda\nabla F(x)) - B^\dagger e)$$

\[= \lambda^{-1}(x + (I - B^\dagger B)\lambda\nabla F(x) - [(I - B^\dagger B)x + B^\dagger e])
\]

\[= \lambda^{-1}(x - \text{Proj}_{\mathcal{X}}(x)) + (I - B^\dagger B)\nabla F(x)
\]

\[= (I - B^\dagger B)\nabla F(x)
\]

where the first equality is due to $\mathcal{X} = \{x | Bx = e\}$ and (29) the last two equality holds since $x \in \mathcal{X}$ and (29). Then with $(I - B^\dagger B)^2 = I - B^\dagger B$ and the definition of $\|\cdot\|_{P_x}$, the proof is complete.

We restate Lemma 2 and Lemma 3 together in a more formal way.

**Restatement of Lemma 2-3.** Under Assumption 1–2 and 4, the gradient of $y^*(x)$ can be expressed as

$$\nabla y^*(x) = -V_2(V_2^T \nabla_{yy}g(x, y^*(x))V_2)^{-1}V_2^T (\nabla_{yx}g(x, y^*(x)) - \nabla_{yy}g(x, y^*(x))A^\dagger \nabla h(x)) = -A^\dagger \nabla h(x)$$

where $V_2$ is the orthogonal basis of $\text{Ker}(A) := \{y \mid Ay = 0\}$. Moreover, $y^*(x)$ is $L_y$ Lipschitz continuous and $L_{yx}$ smooth with

\begin{align*}
L_y := \frac{\ell_{g,1} + (\ell_{g,1} + \mu_g)\|A^\dagger\|\ell_{h,0}}{\mu_g}, \\
L_{yx} := \frac{\ell_{g,2} (1 + \|A^\dagger\|\ell_{h,0}) (1 + L_y)(1 + \frac{\ell_{g,1}}{\mu_g}) + (\ell_{g,1} + \mu_g)\|A^\dagger\|\ell_{h,1}}{\mu_g}
\end{align*}

(31)
Proof: By singular value decomposition, we can decompose $A = U \Sigma V^\top$ with $\Sigma = \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{m_y \times d_y}$, and orthogonal matrix $U = [U_1 \ U_2] \in \mathbb{R}^{m_y \times m_y}$ and $V = [V_1 \ V_2] \in \mathbb{R}^{d_y \times d_y}$. Also, by assuming $\text{Rank}(A) = r$, we know that $U_1 \in \mathbb{R}^{m_y \times r}$, $V_1 \in \mathbb{R}^{d_y \times r}$ and $\Sigma_1 \in \mathbb{R}^{r \times r}$ are full rank submatrix. Therefore, $A$ can be decomposed by

$$A = [U_1 \ U_2] \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1^\top \\ V_2^\top \end{bmatrix} = [U_1 \Sigma_1 \ 0] \begin{bmatrix} V_1^\top \\ V_2^\top \end{bmatrix} = U_1 \Sigma_1 V_1^\top$$

and $V_2$ is the orthogonal basis of $\text{Ker}(A)$.

Next, if we define $y_0(x) := A^\top(c - h(x))$, we can prove $y_0(x) \in \mathcal{Y}(x)$ since

$$Ay_0(x) = AA^\top(c - h(x)) = c - h(x)$$

where the last equality holds due to Assumption 4. From the definition of $y_0(x)$ and (26), we know

$$\nabla_x y_0(x) = -A^\top \nabla h(x). \quad (32)$$

Moreover, since $V_2$ is the orthogonal basis of $\text{Ker}(A)$, we know $\mathcal{Y}(x) = y_0(x) + \text{Ran}(V_2)$. Thus, let $z^*(x) = \arg \min_z g(x, y_0(x) + V_2 z)$, then we have $y^*(x) = y_0(x) + V_2 z^*(x)$.

Since $z^*(x)$ satisfies

$$\nabla_z g(x, y_0(x) + V_2 z^*(x)) = V_2^\top \nabla_y g(x, y_0(x) + V_2 z^*(x)) = 0$$

then taking the gradient with respect to $x$ of both sides, we get

$$0 = \nabla_x (V_2^\top \nabla_y g(x, y_0(x) + V_2 z^*(x)))$$

$$= \nabla_{xy} g(x, y_0(x) + V_2 z^*(x)) V_2 + \left(\nabla_x z^*(x)^\top V_2^\top + \nabla_x y_0(x)^\top\right) \nabla_{yy} g(x, y_0(x) + V_2 z^*(x)) V_2$$

$$= \nabla_{xy} g(x, y_0(x) + V_2 z^*(x)) V_2 + \left(\nabla_x z^*(x)^\top V_2^\top - \nabla^\top h(x) A^\top\right) \nabla_{yy} g(x, y_0(x) + V_2 z^*(x)) V_2$$

$$= \nabla_{xy} g(x, y_0(x) + V_2 z^*(x)) V_2 + \left(\nabla_x z^*(x)^\top V_2^\top - \nabla^\top h(x) A^\top\right) \nabla_{yy} g(x, y_0(x) + V_2 z^*(x)) V_2 \quad (33)$$

where the third equality holds from (32). Then, rearranging (33), we get

$$\nabla z^*(x) = - \left( V_2^\top \nabla_{yy} g(x, y_0(x) + V_2 z^*(x)) V_2 \right)^{-1} V_2^\top \left( \nabla_{yx} g(x, y^*(x)) - \nabla_{yy} g(x, y^*(x)) A^\top \nabla h(x) \right) \quad (34)$$

and as a result of $y^*(x) = y_0(x) + V_2 z^*(x)$, we have

$$\nabla y^*(x) = \nabla y_0(x) + V_2 \nabla z^*(x)$$

$$= -A^\top \nabla h(x) - V_2 \left( V_2^\top \nabla_{yy} g(x, y^*(x)) V_2 \right)^{-1} V_2^\top \left( \nabla_{yx} g(x, y^*(x)) - \nabla_{yy} g(x, y^*(x)) A^\top \nabla h(x) \right). \quad (35)$$

Next, utilizing the fact that $V_2$ is the orthogonal matrix, we know $\mu g I_{d_y - r} \preceq V_2^\top \nabla_{yy} g(x, y) V_2$. Therefore, we have for any $x, y$,

$$V_2 \left( V_2^\top \nabla_{yy} g(x, y) V_2 \right)^{-1} V_2^\top \preceq \frac{1}{\mu g} I. \quad (36)$$

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Besides, we have for any $x$, it follows that
\[
\|\nabla_{yx} g(x, y^*(x)) - \nabla_{yy} g(x, y^*(x))\| A^\top \nabla h(x) \| \leq (1 + \| A^\top \| \ell_{h,0}) \| \nabla^2 g(x, y^*(x)) \|
\leq (1 + \| A^\top \| \ell_{h,0}) \ell_{g,1.}
\] (37)

As a result of (35), (36) and (37), $\nabla y^*(x)$ is bounded by
\[
\|\nabla y^*(x)\|
\leq \left\| V_2 \left( V_2^\top \nabla_{yy} g(x, y^*(x)) V_2 \right)^{-1} V_2^\top \right\| \| \nabla_{yx} g(x, y^*(x)) - \nabla_{yy} g(x, y^*(x))\| A^\top \nabla h(x) \| + \| A^\top \nabla h(x) \|
\leq \frac{\ell_{g,1} + (\ell_{g,1} + \mu_g)}{\mu_g} \| A^\top \| \ell_{h,0} = L_y
\]

which implies $y^*(x)$ is $L_y$ Lipschitz continuous.

Finally, we aim to prove the smoothness of $y^*(x)$. Defining $B_1 = V_2^\top \nabla_{yy} g(x_1, y^*(x_1)) V_2$ and $B_2 = V_2^\top \nabla_{yy} g(x_2, y^*(x_2)) V_2$, for any $x_1$ and $x_2$, we have
\[
\|\nabla y^*(x_1) - \nabla y^*(x_2)\|
= \left\| V_2 \left( V_2^\top \nabla_{yy} g(x_1, y^*(x_1)) V_2 \right)^{-1} V_2^\top \left( \nabla_{yx} g(x_1, y^*(x_1)) \right) - \nabla_{yy} g(x_1, y^*(x_1))\| A^\top \nabla h(x_1) \right\|
\leq \left\| V_2 B_1^{-1} V_2^\top \nabla_{yx} g(x_1, y^*(x_1)) \| - \nabla_{yx} g(x_2, y^*(x_2))\| \right\|
+ \left\| V_2 B_1^{-1} V_2^\top \nabla_{yy} g(x_1, y^*(x_1))\| A^\top \nabla h(x_1) \| - \nabla_{yy} g(x_2, y^*(x_2))\| A^\top \nabla h(x_2) \right\|
\leq \left( 1 + \| A^\top \| \ell_{h,0} \right) L_y \left( 1 + \frac{\ell_{g,1}}{\mu_g} \right)
\leq \frac{\ell_{g,2} \left( 1 + \| A^\top \| \ell_{h,0} \right) (1 + L_y) \left( 1 + \ell_{g,1} / \mu_g \right) A^\top \| \ell_{h,0} A^\top \| \| \ell_{h,0} A^\top \| \| \ell_{h,0} A^\top \| \| x_1 - x_2 \right\|
\] (38)

where (a) comes from (36), (37) and the following fact
\[
V_2 \left( B_1^{-1} - B_2^{-1} \right) V_2^\top
= V_2 \left( B_1^{-1} (B_2 - B_1) B_2^{-1} V_2^\top \right)
= V_2 \left( B_1^{-1} \left( \left( V_2^\top \nabla_{yy} g(x_2, y^*(x_2)) V_2 \right) - \left( V_2^\top \nabla_{yy} g(x_1, y^*(x_1)) V_2 \right) \right) \right) B_2^{-1} V_2^\top
= V_2 \left( B_1^{-1} V_2^\top \left( \nabla_{yy} g(x_2, y^*(x_2)) - \nabla_{yy} g(x_1, y^*(x_1)) \right) \right) V_2 B_2^{-1} V_2^\top
\]
so that
\[
\|V_2 (B_1^{-1} - B_2^{-1}) V_2^T \| \leq \|V_2 B_1^{-1} V_2^T \| \| \nabla_{yy} g(x_2, y^*(x_2)) - \nabla_{yy} g(x_1, y^*(x_1)) \| \|V_2 B_2^{-1} V_2^T \|
\]
\[
\leq \frac{1}{\mu^2} \| \nabla_{yy} g(x_2, y^*(x_2)) - \nabla_{yy} g(x_1, y^*(x_1)) \|
\]
(39)
and (b) comes from
\[
\|\nabla^2 g(x_1, y^*(x_1)) - \nabla^2 g(x_2, y^*(x_2))\| \leq \ell_{g,2} \|x_1 - x_2\| + \|y^*(x_1) - y^*(x_2)\|
\]
\[
\leq \ell_{g,2} (1 + L_y) \|x_1 - x_2\|
\]
from which the proof is complete.  

A.2 Supporting lemmas

Lemma 7. Under Assumption 1–2 and 4, \( F(x) \) is smooth with constant \( L_F \) which is defined as
\[
L_F := \ell_{f,1} (1 + L_y)^2 + \ell_{f,0} L_{yx}.
\]

Proof: For any \( x_1 \) and \( x_2 \), we have that
\[
\| \nabla F(x_1) - \nabla F(x_2) \| = \| \nabla_x f(x_1, y^*(x_1)) + \nabla^\top y^*(x_1) \nabla_y f(x_1, y^*(x_1)) \\
- \nabla_x f(x_2, y^*(x_2)) + \nabla^\top y^*(x_2) \nabla_y f(x_2, y^*(x_2)) \|
\]
\[
\leq \| \nabla_x f(x_1, y^*(x_1)) - \nabla_x f(x_2, y^*(x_2)) \|
\]
\[
+ \| \nabla^\top y^*(x_1) \nabla_y f(x_1, y^*(x_1)) - \nabla^\top y^*(x_2) \nabla_y f(x_2, y^*(x_2)) \|
\]
\[
\leq \ell_{f,1} \|x_1 - x_2\| + \|y^*(x_1) - y^*(x_2)\|
\]
\[
+ \| \nabla y^*(x_1) \| \| \nabla y f(x_1, y^*(x_1)) - \nabla y f(x_2, y^*(x_2)) \|
\]
\[
+ \| \nabla y f(x_2, y^*(x_2)) \| \| \nabla y^*(x_1) - \nabla y^*(x_2) \|
\]
\[
\leq (a) \left( \ell_{f,1} (1 + L_y)^2 + \ell_{f,0} L_{yx} \right) \|x_1 - x_2\| = L_F \|x_1 - x_2\|
\]
where (a) comes from the Lipschitz continuity of \( y^*(x) \), \( \nabla y^*(x) \) in Lemma 3 and the Lipschitz continuity of \( \nabla f \) and \( f \) in Assumption 1.  

For simplicity, we denote
\[
\nabla f(x, y) = \nabla_x f(x, y) + \left( \left( \nabla h(x)^\top A^{\top} \nabla_{yy} g(x, y) - \nabla_{xy} g(x, y) \right) \right)
\times V_2 (V_2^\top \nabla_{yy} g(x, y) V_2)^{-1} V_2^\top - \nabla h(x)^\top A^{\top} \right) \nabla_y f(x, y).
\]

(42)

Lemma 8 (Boundness of \( \nabla f(x, y) \)). Under Assumption 1–2, for any \( x, y \), \( \| \nabla f(x, y) \| \leq \ell_{f,0} (1 + L_y) \).

Proof: Based on (36), we have that
\[
\| V_2 \left( V_2^\top \nabla_{yy} g(x, y) V_2 \right)^{-1} V_2^\top \| \leq \frac{1}{\mu^2}.
\]

(43)
Then we can obtain the bound for $\nabla f(x, y)$ since
\[
\| \nabla f(x, y) \| \leq \| \nabla x f(x, y) \| + \| \nabla h(x)^T A^T \nabla y g(x, y) - \nabla y g(x, y) \| \\
\times \| V_2 (V_2^T \nabla y g(x, y) V_2)^{-1} V_2^T \| \| \nabla y f(x, y) \| + \| \nabla h(x)^T A^T \| \| \nabla y f(x, y) \|
\]
\[
\leq \ell_{f, 0} \left( 1 + \ell_{g, 1} \frac{\ell_{f, 1} + \ell_{f, 0} \ell_{g, 2}}{\mu_g} + \ell_{h, 0} \| A^T \| \right) \leq \ell_{f, 0} (1 + L_y)
\]
from which the proof is complete.

\[\text{Lemma 9 (Lipschitz continuity of } \nabla f(x, y)\text{). Under Assumption I–2 and 4, } \nabla f(x, y) \text{ is } L_f \text{ Lipschitz continuous with respect to } y, \text{ where the constant is defined as}
\]
\[
L_f := \left( 1 + \ell_{h, 0} \| A^T \| \right) \left( \ell_{f, 1} + \frac{\ell_{g, 1} \ell_{f, 1} + \ell_{f, 0} \ell_{g, 2}}{\mu_g} + \frac{\ell_{f, 0} \ell_{g, 1} \ell_{g, 2}}{\mu_g^2} \right).
\]

\[\text{Proof: For simplicity, we define some notations first.}
\]
\[
B_1 = V_2^T \nabla y g(x, y_1) V_2, \quad B_2 = V_2^T \nabla y g(x, y_2) V_2,
\]
\[
C_1 = \nabla h(x)^T A^T \nabla y g(x, y_1) - \nabla y g(x, y_1),
\]
\[
C_2 = \nabla h(x)^T A^T \nabla y g(x, y_2) - \nabla y g(x, y_2).
\]

For $i = 1, 2$, according to (36), we have the following bounds.
\[
\| C_i \| \leq \left( 1 + \ell_{h, 0} \| A^T \| \right) \ell_{g, 1}, \quad \| V_2 B_1^{-1} V_2^T \| \leq \frac{1}{\mu_g}, \quad \| \nabla y f(x, y_i) \| \leq \ell_{f, 0}.
\]

Besides, we can also bound their differences as
\[
\| C_1 - C_2 \| \leq \left( 1 + \| A^T \| \ell_{h, 0} \right) \| \nabla^2 g(x, y_1) - \nabla^2 g(x, y_2) \| \leq \left( 1 + \| A^T \| \ell_{h, 0} \right) \ell_{g, 2} \| x_1 - x_2 \|
\]
and
\[
\| V_2 B_1^{-1} V_2^T - V_2 B_2^{-1} V_2^T \| \overset{(a)}{=} \| V_2 B_1^{-1} V_2^T \| \| V_2 B_2^{-1} V_2^T \| \| \nabla y g(x, y_1) - \nabla y g(x, y_2) \|
\]
\[
\leq \frac{\ell_{g, 2}}{\mu_g^2} \| y_1 - y_2 \|
\]
where (a) is due to
\[
V_2 (B_1^{-1} - B_2^{-1}) V_2^T
\]
\[
= V_2 B_1^{-1} (B_2 - B_1) B_2^{-1} V_2^T
\]
\[
= V_2 B_1^{-1} \left( \left( V_2^T \nabla y g(x, y_2) V_2 \right) - \left( V_2^T \nabla y g(x, y_1) V_2 \right) \right) B_2^{-1} V_2^T
\]
\[
= V_2 B_1^{-1} V_2^T \left( \nabla y g(x, y_2) - \nabla y g(x, y_1) \right) V_2 B_2^{-1} V_2^T.
\]

Likewise, we have
\[
\| \nabla y f(x, y_1) - \nabla y f(x, y_2) \| \leq \ell_{f, 1} \| x_1 - x_2 \|.
\]
Thus, for any \( x, y_1, y_2 \), based on (45) and (47), we have
\[
\| \nabla f(x, y_1) - \nabla f(x, y_2) \|
\leq \| \nabla_x f(x, y_1) - \nabla_x f(x, y_2) \| + \| C_1 V_2 B_1^{-1} V_2^T \nabla_y f(x, y_1) - C_2 V_2 B_2^{-1} V_2^T \nabla_y f(x, y_2) \|
\leq \| \nabla h(x) \| \| A^\dagger \| \| \nabla_y f(x, y_1) - \nabla_y f(x, y_2) \|
\leq (1 + \ell_{h,0} \| A^\dagger \| ) \ell_{f,1} \| y_1 - y_2 \| + \| C_1 \| \| V_2 B_1^{-1} V_2^T \| \| \nabla_x f(x, y_1) - \nabla_x f(x, y_2) \|
\leq (1 + \ell_{h,0} \| A^\dagger \| ) \left( \ell_{f,1} + \frac{\ell_{f,0} \ell_{g,2}}{\mu_y} + \frac{\ell_{f,0} \ell_{g,1} \ell_{g,2}}{\mu_y^2} \right) \| y_1 - y_2 \|
\] (48)

where (a) is due to
\[
\begin{align*}
C_1 D_1 E_1 & - C_2 D_2 E_2 \\
= & C_1 D_1 E_1 - C_1 D_1 E_2 + C_1 D_1 E_2 - C_1 D_2 E_2 + C_1 D_2 E_2 - C_2 D_2 E_2 \\
= & C_1 D_1 (E_1 - E_2) + C_1 E_2 (D_1 - D_2) + D_2 E_2 (C_1 - C_2)
\end{align*}
\] (49)

(b) comes from (45) and (47), from which the proof is complete.

B Theoretical Analysis for AiPOD

In this section, we present the proof of Algorithm 1. We define
\[
\mathcal{F}_k^s := \sigma\{y^0, x^0, \ldots, y^k, x^k, y^{k,1}, \ldots, y^{k,s}\}
\] (50)

where \( \sigma\{\cdot\} \) denotes the \( \sigma \)-algebra generated by the random variables. Then it follows that \( \mathcal{F}_k^s = \sigma\{y^0, x^0, \ldots, y^{k+1}\} \).

B.1 Supporting lemmas of Theorem 1

To prove the bias and variance of gradient estimator \( h_k^f \), we leverage the following fact.

Lemma 10 ([29, Lemma 12]). Let \( Z_i \) be a sequence of stochastic matrices defined recursively as \( Z_i = Y_i Z_{i-1}, i \geq 0 \) with \( Z_{-1} = I \in \mathbb{R}^{d \times d} \). \( Y_i \) are independent, symmetric random matrix satisfying
\[
\| \mathbb{E} [Y_i] \| \leq 1 - \mu, \quad \mathbb{E} \left[ \| Y_i - \mathbb{E} [Y_i] \| ^2 \right] \leq \sigma^2.
\]

If \( (1 - \mu)^2 + \sigma^2 < 1 \), then for any \( i > 0 \), it holds that
\[
\mathbb{E} \left[ \| Z_i \| ^2 \right] \leq d ((1 - \mu)^2 + \sigma^2)^i.
\]

Based on this lemma, we can bound the second moment bound of Hessian inverse estimator.
Lemma 11. Under Assumption 1–4, let \( \tilde{c} = \frac{\mu_g}{\mu_g^2 + \sigma_g^2} \) and for any \( k \), denote the Hessian inverse estimator as

\[
H_{yy}^k = \frac{\tilde{c}N}{\ell_g,1} \prod_{n=0}^{N'} \left( I - \frac{\tilde{c}}{\ell_g,1} V_2^T \nabla_{yy} g \left( x^k, y^{k+1}; \phi_{(n)} \right) V_2 \right).
\]

With \( r = \text{Rank}(A) \), the second moment bound of \( H_{yy}^k \) can be bounded as

\[
\mathbb{E} \left[ \| H_{yy}^k \|^2 | F_k^S \right] \leq \frac{N(d_y - r)}{\ell_g,1 (\mu_g^2 + \sigma_g^2)}.
\]

Proof: Letting \( Y_n = I - \frac{\tilde{c}}{\ell_g,1} V_2^T \nabla_{yy} g \left( x, \phi_{(n)} \right) V_2 \), it follows that

\[
\| E[Y_n] \| \leq \left( 1 - \frac{\tilde{c} \mu_g}{\ell_g,1} \right), \quad \mathbb{E} \left[ \| Y_n - E[Y_n] \|^2 \right] \leq \frac{\tilde{c}^2 \sigma_g^2}{\ell_g,1^2}.
\]

Moreover, since

\[
\left( 1 - \frac{\tilde{c} \mu_g}{\ell_g,1} \right)^2 + \frac{\tilde{c}^2 \sigma_g^2}{\ell_g,1^2} = 1 - \frac{2 \tilde{c} \mu_g}{\ell_g,1} + \frac{\tilde{c}^2 (\mu_g^2 + \sigma_g^2)}{\ell_g,1} = 1 - \frac{\mu_g^2}{\ell_g,1 (\mu_g^2 + \sigma_g^2)} < 1
\]

which satisfies the condition in Lemma 10, we can then plug \( Y_n \) into Lemma 10 and achieves the second moment bound for \( H_{yy}^k \).

\[
\mathbb{E} \left[ \| H_{yy}^k \|^2 | F_k^S \right] = \mathbb{E} \left[ \mathbb{E} \left[ \| H_{yy}^k \|^2 | N', F_k^S \right] | F_k^S \right] \leq \mathbb{E} \left[ \frac{\tilde{c}^2 N^2 (d_y - r)}{\ell_g,1^2} \left( 1 - \frac{\mu_g^2}{\ell_g,1 (\mu_g^2 + \sigma_g^2)} \right)^n \right] \leq \frac{\tilde{c}^2 N (d_y - r)}{\ell_g,1 (\mu_g^2 + \sigma_g^2)}.
\]

where \( r \) is rank of \( A \) and (a) comes from the choice of \( \tilde{c} \).

Lemma 12 (Bias and variance of gradient estimator). Let \( \tilde{c} = \frac{\mu_g}{\mu_g^2 + \sigma_g^2}, r = \text{rank}(A) \) and define

\[
\tilde{h}_f^k = \mathbb{E} \left[ h_f^k | F_k^S \right],
\]

then \( \tilde{h}_f^k \) is a biased estimator of UL gradient which satisfies that

\[
\| \tilde{h}_f^k - \nabla f(x^k, y^{k+1}) \| \leq L_y \ell_{f,0} \left( 1 - \frac{\mu_g^2}{\ell_g,1 (\mu_g^2 + \sigma_g^2)} \right)^N =: b_k
\]

\[
\mathbb{E} \left[ H_{yy}^k - \tilde{h}_f^k \right] \leq (1 + \ell_{h,0} \| A^\dagger \|) \sigma_f^2 + \frac{4 N (1 + \ell_{h,0}^2 \| A^\dagger \|^2) (d_y - r)(\ell_{f,0}^2 + \sigma_g^2)(2 \sigma_g^2 + \ell_{f,0}^2)}{\ell_g,1 (\mu_g^2 + \sigma_g^2)} =: \sigma_f^2 = O(N).
\]
Proof: We first prove (51) by noticing that the error by finite updates can be bounded by

\[
\left\| V_2 \left( (I - D)^{-1} - \sum_{n=0}^{N-1} D^n \right) V_2^T \right\| = \left\| V_2 \left( \sum_{n=N}^{\infty} D^n \right) V_2^T \right\| = \left\| \sum_{n=N}^{\infty} (V_2 D V_2^T)^n \right\| \\
\leq \sum_{n=N}^{\infty} \|V_2 D V_2^T\|^n = \frac{\|V_2 D V_2^T\|^N}{1 - \|V_2 D V_2^T\|} \quad (53)
\]

Thus, letting \( D = I - \frac{\bar{c}}{\ell_{g,1}} V_2^T \nabla_{yy} g(x, y) V_2 \) and multiplying each side by \( \frac{\bar{c}}{\ell_{g,1}} \), we obtain that

\[
\left\| V_2 \left( \left( V_2^T \nabla_{yy} g(x, y) V_2 \right)^{-1} - \frac{\bar{c}}{\ell_{g,1}} \sum_{n=0}^{N-1} \left( I - \frac{\bar{c}}{\ell_{g,1}} V_2^T \nabla_{yy} g(x, y) V_2 \right)^n \right) V_2^T \right\| \leq \frac{\bar{c}^2 \ell_{g,1}}{\ell_{g,1} (1 - \|V_2 \left( I - \frac{\bar{c}}{\ell_{g,1}} V_2^T \nabla_{yy} g(x, y) \right) V_2^T \|)} \leq \left( 1 - \frac{\bar{\mu}_g}{\ell_{g,1}} \right)^N \quad (54)
\]

where the second inequality holds according to \( \mu_g I_{d_y-r} \leq V_2^T \nabla_{yy} g(x, y) V_2 \). Then we have

\[
\| \nabla f(x^k, y^{k+1}) - \tilde{h}_f \| \leq \left\| \nabla h(x^0)^T A^T \nabla_{yy} g(x^k, y^{k+1}) - \nabla_{xy} g(x^k, y^{k+1}) \right\| \| \nabla_y f(x^k, y^{k+1}) \| \\
\times \left\| V_2 \left( \left( V_2^T \nabla_{yy} g(x^k, y^{k+1}) V_2 \right)^{-1} - \frac{\bar{c}}{\ell_{g,1}} \sum_{n=0}^{N-1} \left( I - \frac{\bar{c}}{\ell_{g,1}} V_2^T \nabla_{yy} g(x, y) V_2 \right)^n \right) V_2^T \right\| \leq \left( 1 + \ell_{h,0} \|A^T\| \| \ell_{g,1} \ell_{f,0} \left( 1 - \frac{\bar{\mu}_g}{\ell_{g,1}} \right)^N \right) \leq L_y \ell_{f,0} \left( 1 - \frac{\bar{\mu}_g}{\ell_{g,1}} \right)^N \quad (55)
\]

where the second term of (a) is derived from \( \|X^{-1} - Y^{-1}\| \leq \|X^{-1}\| \|X - Y\| \|Y^{-1}\| \). Then plugging in the choice of \( \bar{c} \) to (55) results in (51).

The proof of (52) is based on Lemma 11. For ease of narration, we denote

\[
\nabla_{xy}^h g(x^k, y^{k+1}; \phi_{(0)}):= \nabla h(x^k)^T A^T \nabla_{yy} g(x^k, y^{k+1}; \phi_{(0)}) - \nabla_{xy} g(x^k, y^{k+1}; \phi_{(0)}) \\
\nabla_{xy}^h g(x^k, y^{k+1}):= \nabla h(x^k)^T A^T \nabla_{yy}^2 g(x^k, y^{k+1}) - \nabla_{xy}^2 g(x^k, y^{k+1}).
\]

We notice that

\[
E \left[ \nabla_{xy}^h g(x^k, y^{k+1}; \phi_{(0)}), F_k^S \right] = \nabla_{xy}^h g(x^k, y^{k+1})
\]

and then the bias and variance of \( \nabla_{xy}^h g(x^k, y^{k+1}; \phi_{(0)}) \) can be bounded by

\[
\| \nabla_{xy}^h g(x^k, y^{k+1}) \|^2 \leq 2(1 + \ell_{h,0}^2 \|A^T\|^2) \ell_{g,1}^2 \quad (56)
\]
Thus adding (56) and (57), we arrive at the second moment bound for $\nabla_{xy}^h g(x^k, y^{k+1}; \phi^k(0))$ as

$$
E \left[ \| \nabla_{xy}^h g(x^k, y^{k+1}; \phi^k(0)) - \nabla_{xy}^h g(x^k, y^{k+1}) \|^2 \right]
\leq \| \nabla h(x^k)^T A^T \|^2 E \left[ \| \nabla_{yy} g(x^k, y^{k+1}; \phi^k(0)) - \nabla_{yy} g(x^k, y^{k+1}) \|^2 \right]
+ E \left[ \| \nabla_{xy} g(x^k, y^{k+1}; \phi^k(0)) - \nabla_{xy} g(x^k, y^{k+1}) \|^2 \right]
\leq (1 + \ell_{h,0}^2 \| A \|^2) \sigma_{g,2}^2. \tag{57}
$$

Thus adding (56) and (57), we arrive at the second moment bound for $\nabla_{xy}^h g(x^k, y^{k+1}; \phi^k(0))$ as

$$
E \left[ \| \nabla_{xy}^h g(x^k, y^{k+1}; \phi^k(0)) \|^2 \right]
= E \left[ \| \nabla_{xy}^h g(x^k, y^{k+1}; \phi^k(0)) \|^2 \right] + E \left[ \| \nabla_{xy}^h g(x^k, y^{k+1}; \phi^k(0)) - \nabla_{xy}^h g(x^k, y^{k+1}) \|^2 \right]
\leq (1 + \ell_{h,0}^2 \| A \|^2)(2\sigma_{g,2}^2 + \sigma_{g,2}^2).
$$

Then the variance of $h^k_f$ can be decomposed and bounded as

$$
E \left[ \| h^k_f - h^k_f \|^2 \right]
\leq E \left[ \| \nabla_x f(x^k, y^{k+1}; \xi^k) - \nabla_x f(x^k, y^{k+1}) \|^2 \right]
+ E \left[ \| \nabla h(x^k) A^T \| \| \nabla_y f(x^k, y^{k+1}; \xi^k) - \nabla_y f(x^k, y^{k+1}) \|^2 \right]
+ E \left[ \| \nabla_{xy}^h g(x^k, y^{k+1}; \phi^k(0)) V_2 H_{yy} V_2^T \nabla_y f(x^k, y^{k+1}; \xi^k) \right]
\leq (1 + \ell_{h,0}^2 \| A \|^2) \sigma^2_f.
$$

Then the variance of $h^k_f$ can be decomposed and bounded as

$$
E \left[ \| h^k_f - h^k_f \|^2 \right]
\leq 2E \left[ \| \nabla_{xy}^h g(x^k, y^{k+1}; \phi^k(0)) \|^2 \right] E \left[ \| H_{yy} \|^2 \right] E \left[ \| \nabla_y f(x^k, y^{k+1}; \xi^k) - \nabla_y f(x^k, y^{k+1}) \|^2 \right]
+ E \left[ \| H_{yy} \|^2 \right] E \left[ \| \nabla_y f(x^k, y^{k+1}; \xi^k) \|^2 \right]
\leq (1 + \ell_{h,0}^2 \| A \|^2) \sigma^2_f.
$$

where (a) comes from (49) and $(A + B + C)^2 \leq 3(A^2 + B^2 + C^2)$, and (b) comes from the second moment bound and variance of $\nabla_{xy}^h g(x^k, y^{k+1}; \phi^k(0))$, $H_{yy}$ and $\nabla_y f(x^k, y^{k+1}; \xi^k)$. \hfill \blacksquare

### B.2 Descent of upper and lower levels

**Lemma 13 (Descent of upper level).** Suppose Assumption 1–4 hold, then the sequence of $x_k$ generated by Algorithm 1 satisfies

$$
E[F(x^{k+1})] - E[F(x^k)] \leq -\frac{\alpha}{2} E \left[ \| \nabla F(x^k) \|^2 \right] + \alpha L_{F}^2 E \left[ \| y^*(x^k) - y^{k+1} \|^2 \right] + \alpha b_{k}^2
- \left( \frac{\alpha}{2} - \frac{L_{F} \alpha^2}{2} \right) E \left[ \| \tilde{h}^k_f \|^2 \right] + \frac{L_{F} \alpha^2 \sigma_f^2}{2}, \tag{59}
$$

where $P_x = I - B^\dagger B$ is the projection matrix of $B$ and $B^\dagger$ is the Moore-Penrose inverse of $B$.\hfill \blacksquare
Proof: Since $\mathcal{X} = \{x \mid Bx = e\}$, for any $x$, we have that $\text{Proj}_{\mathcal{X}}(x) = (I - B^\dagger B)x + B^\dagger e$ is a linear operator of $x$ according to (29). Thus, we have

$$x^{k+1} = \text{Proj}_{\mathcal{X}}(x^k - \alpha h_f^k) = (I - B^\dagger B)(x^k - \alpha h_f^k) + B^\dagger e$$
$$= (I - B^\dagger B)x^k + B^\dagger e - (I - B^\dagger B)(\alpha h_f^k)$$
$$= \text{Proj}_{\mathcal{X}}(x^k) - \alpha (I - B^\dagger B)h_f^k$$
$$= x^k - \alpha (I - B^\dagger B)h_f^k$$  \hspace{1cm} (60)

where the last equality is due to $x^k \in \mathcal{X}$.

Taking the expectation of $F(x^{k+1})$ conditioned on $\mathcal{F}_k^S$, we get

$$\mathbb{E}\left[F(x^{k+1})|\mathcal{F}_k^S\right] \overset{(a)}{\leq} F(x^k) + \langle \nabla F(x^k), \mathbb{E}\left[x^{k+1} - x^k | \mathcal{F}_k^S\right]\rangle + \frac{L_F}{2}\mathbb{E}\left[\|x^{k+1} - x^k\|^2 | \mathcal{F}_k^S\right]$$
$$= F(x^k) - \alpha \langle \nabla F(x^k), (I - B^\dagger B)\tilde{h}_f^k\rangle + \frac{L_F}{2}\alpha^2\mathbb{E}\left[\| (I - B^\dagger B)\|\tilde{h}_f^k\|^2 | \mathcal{F}_k^S\right]$$
$$\overset{(b)}{\leq} F(x^k) - \frac{\alpha}{2}\| (I - B^\dagger B)\nabla F(x^k)\|^2 + \frac{\alpha}{2}\| (I - B^\dagger B)(\nabla F(x^k) - \tilde{h}_f^k)\|^2$$
$$- \left(\frac{\alpha}{2} - \frac{L_F\alpha^2}{2}\right)\| (I - B^\dagger B)\tilde{h}_f^k\|^2 + \frac{L_F\alpha^2\sigma_f^2}{2}$$
$$\overset{(c)}{\leq} F(x^k) - \frac{\alpha}{2}\| \nabla F(x^k)\|^2_{\mathbb{P}_x} + \frac{\alpha}{2}\| \nabla F(x^k) - \tilde{h}_f^k\|^2$$
$$- \left(\frac{\alpha}{2} - \frac{L_F\alpha^2}{2}\right)\| \tilde{h}_f^k\|^2_{\mathbb{P}_x} + \frac{L_F\alpha^2\sigma_f^2}{2}$$  \hspace{1cm} (61)

where (a) comes from the smoothness of $F$, (b) is derived from $2a^\top b = \|a\|^2 + \|b\|^2 - \|a - b\|^2$, $\mathbb{E}[\|X\|^2|Y] = \mathbb{E}[\|X\|^2] + \mathbb{E}[\|X - \mathbb{E}[X|Y]\|^2|Y]$, $(I - B^\dagger B)^2 = I - B^\dagger B$ and Lemma 12, (c) is due to the definition of $\| \cdot \|_{\mathbb{P}_x}$ and $\| (I - B^\dagger B)\| \leq 1$.

Besides, we decompose the gradient bias term as follows

$$\| \nabla F(x^k) - \tilde{h}_f^k\|^2 \leq 2\| \nabla F(x^k) - \nabla f(x^k, y^{k+1})\|^2 + 2\| \nabla f(x^k, y^{k+1}) - \tilde{h}_f^k\|^2$$
$$\leq 2\| \nabla f(x^k, y^*(x^k)) - \nabla f(x^k, y^{k+1})\|^2 + 2\sigma_f^2$$
$$\leq 2L_f^2\| y^*(x^k) - y^{k+1}\|^2 + 2\sigma_f^2$$  \hspace{1cm} (62)

Plugging (62) to (61) and taking expectation, we get that

$$\mathbb{E}[F(x^{k+1})] - \mathbb{E}[F(x^k)] \leq -\frac{\alpha}{2}\mathbb{E}\left[\| \nabla F(x^k)\|^2_{\mathbb{P}_x}\right] + \alpha L_f^2\mathbb{E}\left[\| y^*(x^k) - y^{k+1}\|^2\right] + \alpha \sigma_f^2$$
$$- \left(\frac{\alpha}{2} - \frac{L_F\alpha^2}{2}\right)\mathbb{E}\left[\| \tilde{h}_f^k\|^2_{\mathbb{P}_x}\right] + \frac{L_F\alpha^2\sigma_f^2}{2}.$$  

This completes the proof. \hfill \blacksquare

Lemma 14 (Error of lower-level update). Suppose that Assumption 1–4 hold and $\beta \leq \frac{1}{s\mu_g}$, then the error of lower-level variable can be bounded by

$$\mathbb{E}[\| y^{k+1} - y^*(x^k)\|^2] \leq (1 - \beta \mu_g)^S \mathbb{E}[\| y^k - y^*(x^k)\|^2] + S\beta^2\sigma^2_{g,1}$$  \hspace{1cm} (63a)
\[ \mathbb{E}[\|y^{k+1} - y^*(x^{k+1})\|^2] \leq \left( 1 + \gamma + L_{yx} \bar{C}_f^2 \alpha^2 \right) \mathbb{E}[\|y^{k+1} - y^*(x^k)\|^2] \\
+ \left( L_y^2 + L_{yx} \right) \alpha^2 \sigma_f^2 + \left( L_y^2 + L_{yx} + \frac{L_y^2}{\gamma} \right) \alpha^2 \mathbb{E} \left[ \|h_f^k\|^2 \|P_s\| \right] \] (63b)

where \( \bar{C}_f^2 := 2L_y^2 + 2L_{yx}^2 \left( 1 + \frac{L_y^2}{\mu_y} \right) \) and \( \sigma_f^2 \). \( \gamma \) is parameter which will be chosen in the final theorem.

**Proof:** First, since the lower-level objective function is strongly-convex and smooth, when \( 0 \leq \beta \leq \frac{1}{t_{g,1}} \), we have the following fact

\[
\|y_1 - \beta \nabla_y g(x, y_1) - (y_2 - \beta \nabla_y g(x, y_2))\|^2 \\
= \|y_1 - y_2\|^2 + 2\beta \|\nabla_y g(x, y_1) - \nabla_y g(x, y_2)\|^2 - 2\beta \langle y_1 - y_2, \nabla_y g(x, y_1) - \nabla_y g(x, y_2) \rangle \\
\leq (1 - \beta \mu_y) \|y_1 - y_2\|^2 - 2\beta \|\nabla_y g(x, y_1) - \nabla_y g(x, y_2)\|^2 \\
\leq (1 - \beta \mu_y) \|y_1 - y_2\|^2 
\]

(64)

where the first inequality is according to (27) and the last inequality is due to (28) and \( \beta \leq \frac{1}{t_{g,1}} \).

Then, for each lower-level update, we obtain that

\[
\mathbb{E}[\|y^{k,s+1} - y^*(x^k)\|^2 | \mathcal{F}_{k,s}] \\
= \mathbb{E}[\| \text{Proj}_{\mathcal{Y}(x^k)}(y^{k,s} - \beta \nabla_y g(x^k, y^{k,s}; \phi^k,s)) - \text{Proj}_{\mathcal{Y}(x^k)}(y^*(x^k) - \beta \nabla_y g(x^k, y^*(x^k))) \|^2 | \mathcal{F}_{k}^s] \\
\leq \mathbb{E}[\|y^{k,s} - \beta \nabla_y g(x^k, y^{k,s}; \phi^k,s) - y^*(x^k) + \beta \nabla_y g(x^k, y^*(x^k))\|^2 | \mathcal{F}_{k}^s] \\
\leq \mathbb{E}[\|\nabla_y g(x^k, y^{k,s}; \phi^k,s) - \nabla_y g(x^k, y^*(x^k))\|^2 | \mathcal{F}_{k}^s] \\
+ \beta^2 \mathbb{E}[\|\nabla_y g(x^k, y^{k,s}; \phi^k,s) - \nabla_y g(x^k, y^*(x^k))\|^2 | \mathcal{F}_{k}^s] \\
\leq (1 - \beta \mu_y) \|y^{k,s} - y^*(x^k)\|^2 + 2\beta \sigma_{g,1}^2 
\]

(65)

where the first inequality is due to \( y^*(x^k) = \text{Proj}_{\mathcal{Y}(x^k)}(y^*(x^k) - \beta \nabla_y g(x^k, y^*(x^k))) \), the second inequality is due to Lemma 5 and the last inequality is obtained by (64) with \( x = x^k, y_2 = y^*(x^k), y_1 = y^{k,s} \), and Assumption 3. Taking the expectation of both sides in (65), one has

\[
\mathbb{E}[\|y^{k,s+1} - y^*(x^{k+1})\|^2] \leq (1 - \beta \mu_y) \mathbb{E}[\|y^{k,s} - y^*(x^k)\|^2] + 2\beta \sigma_{g,1}^2. 
\]

(66)

Thus, (63a) can be obtained by telescoping (66).

On the other hand, we have

\[
\|y^{k+1} - y^*(x^{k+1})\|^2 = \|y^{k+1} - y^*(x^k)\|^2 + \underbrace{\|y^*(x^k) - y^*(x^{k+1})\|^2}_{J_1} \\
+ 2 \langle y^{k+1} - y^*(x^k), y^*(x^k) - y^*(x^{k+1}) \rangle_{J_2}.
\]

Since \( y^*(x) \) is \( L_y \) Lipschitz continuous, \( J_1 \) can be bounded by

\[
\mathbb{E}[J_1] \leq L_y^2 \mathbb{E} \left[ \|x^{k+1} - x^k\|^2 \right] \overset{(a)}{=} \alpha^2 L_y^2 \mathbb{E} \left[ \| (I - B^\dagger B) h_f^k \|^2 \right] |\mathcal{F}_{k}^s | \\
\overset{(b)}{=} \alpha^2 L_y^2 \left( \mathbb{E} \left[ \|h_f^k\|^2 | P_s \right] + \sigma_f^2 \right) 
\]

(67)
where (a) comes from (60), (b) holds since $\mathbb{E}[\|C\|^2|D] = \|\mathbb{E}[C|D]\|^2 + \mathbb{E}[\|C - \mathbb{E}[C|D]\|^2|D]$ and Lemma 12.

Moreover, we can decompose $J_2$ by two terms as follows.

$$ J_2 = -\langle y^{k+1} - y^*(x^k), \nabla y^*(x^k)^\top (x^{k+1} - x^k) \rangle_{J_2:1} - \langle y^{k+1} - y^*(x^k), y^*(x^{k+1}) - y^*(x^k) - \nabla y^*(x^k)^\top (x^{k+1} - x^k) \rangle_{J_2:2}. $$

Moreover, the conditional expectation of $J_{2:1}$ can be bounded by

$$ \mathbb{E}[J_{2:1} | \mathcal{F}_k^S] = -\langle y^{k+1} - y^*(x^k), \mathbb{E}[\nabla y^*(x^k)^\top (x^{k+1} - x^k)|\mathcal{F}_k^S] \rangle \leq -\alpha \langle y^{k+1} - y^*(x^k), \nabla y^*(x^k)^\top (I - B^\top B) \bar{h}_f^k \rangle \leq \frac{\gamma}{2} \|y^{k+1} - y^*(x^k)\|^2 + \frac{\alpha^2 L_y^2}{2\gamma} \|\bar{h}_f^k\|_{\mathcal{P}_y}^2 \tag{68} $n$ where (a) comes form Young’s inequality and the boundedness of $\nabla y^*(x^k)$. Then taking expectation of (68), we obtain that

$$ \mathbb{E}[J_{2:1}] \leq \frac{\gamma}{2} \mathbb{E}[\|y^{k+1} - y^*(x^k)\|^2] + \frac{\alpha^2 L_y^2}{2\gamma} \mathbb{E}[\|\bar{h}_f^k\|_{\mathcal{P}_y}^2]. \tag{69} $$

Based on the smoothness of $y^*(x)$ and Jensen inequality, $J_{2:2}$ can be bounded by

$$ \mathbb{E}[J_{2:2}] \leq \mathbb{E}\left[ \|y^{k+1} - y^*(x^k)\| y^*(x^{k+1}) - y^*(x^k) - \nabla y^*(x^k)^\top (x^{k+1} - x^k) \|^2 \right] \leq \frac{L_{yx}}{2} \mathbb{E}\left[ \|y^{k+1} - y^*(x^k)\| \|x^{k+1} - x^k\|^2 \right] \leq \frac{L_{yx} \alpha^2}{2} \mathbb{E}[\|y^{k+1} - y^*(x^k)\|^2 \|h_f^k\|^2] + \frac{L_{yx} \alpha^2}{2} \mathbb{E}\left[ \|h_f^k\|^2 \|\mathcal{P}_y\| \right] \leq \frac{L_{yx} \alpha^2}{2} \mathbb{E}\left[ \|y^{k+1} - y^*(x^k)\|^2 \left( \|h_f^k\|^2 + \sigma_f^2 \right) \right] + \frac{L_{yx} \alpha^2}{2} \left( \mathbb{E}[\|h_f^k\|_{\mathcal{P}_y}^2] + \sigma_f^2 \right) \leq \frac{L_{yx} \alpha^2}{2} \mathbb{E}\left[ \|y^{k+1} - y^*(x^k)\|^2 \left( 2\|h_f^k - \nabla f(x^k, y^{k+1})\|^2 + 2\|\nabla f(x^k, y^{k+1})\|^2 + \sigma_f^2 \right) \right] + \frac{L_{yx} \alpha^2}{2} \left( \mathbb{E}[\|h_f^k\|_{\mathcal{P}_y}^2] + \sigma_f^2 \right) \leq \frac{L_{yx} \alpha^2}{2} \mathbb{E}\left[ \|y^{k+1} - y^*(x^k)\|^2 \right] \leq \frac{L_{yx} \alpha^2}{2} \left( 2\bar{h}_f^2 + 2\ell_f^2 \bar{h}_f^2 \right) \mathbb{E}[\|y^{k+1} - y^*(x^k)\|^2] + \frac{L_{yx} \alpha^2}{2} \left( \mathbb{E}[\|h_f^k\|_{\mathcal{P}_y}^2] + \sigma_f^2 \right) \tag{70} $$

where (a) comes from the update (60), Young’s inequality and $\|h_f^k\|_{\mathcal{P}_y} = \|(I - B^\top B)h_f^k\| \leq \|h_f^k\|$ and (b) holds from Lemma 8 and Lemma 12. Then denoting $\tilde{C}_f^2 := 2\bar{h}_f^2 + 2\ell_f^2 \bar{h}_f^2 + \sigma_f^2$ and combining (67), (69) and (70), we get

$$ \mathbb{E}[\|y^{k+1} - y^*(x^{k+1})\|^2] \leq \left( 1 + \gamma + L_{yx} \tilde{C}_f^2 \alpha^2 \right) \mathbb{E}[\|y^{k+1} - y^*(x^k)\|^2] + \left( L_y^2 + L_{yx} \alpha^2 \sigma_f^2 \right) $n$
+ \left( L_y^2 + L_{yx}^2 + \frac{L_y^2}{\gamma} \right) \alpha^2 \mathbb{E} \left[ \| \bar{h}_k \|_{P_x}^2 \right].

This completes the proof.

\[ \Box \]

### B.3 Proof of Theorem 1

We first restate a formal version of Theorem 1 as follows.

**Restatement of Theorem 1.** Under Assumption 1–4, defining the constants as

\[
\bar{\alpha}_1 = \frac{1}{2L_F + 4L_f L_y + \frac{4L_f L_{yx}}{L_y}}, \quad \bar{\alpha}_2 = \frac{\mu_g}{\ell_{g,1}(5L_f L_y + L_{yx} \bar{C}_f^2)}
\]

and choosing

\[
\alpha = \min \left( \bar{\alpha}_1, \bar{\alpha}_2, \frac{\bar{\alpha}}{\sqrt{K}} \right), \quad \beta = \frac{5L_f L_y + L_{yx} \bar{C}_f^2}{\mu_g} \alpha, \quad N = O(\log K)
\]

then for any \( S \geq 1 \) in Algorithm 1, we have

\[
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \| \nabla F(x_k) \|_{P_x}^2 \right] = O \left( \frac{\log(K)}{\sqrt{K}} \right)
\]

where \( P_x = I - B^\dagger B \) is the projection matrix on \( \text{Ker}(B) \) and \( \| x \|_{P_x} = \sqrt{x^\top P_x x} \) is the weighted Euclidean norm associated with \( P_x \).

**Proof:** According to Lemma 14 and plugging (63b) into (63a), we get that

\[
\mathbb{E} \left[ \| y^{k+1} - y^*(x^{k+1}) \|^2 \right] \leq \left( 1 + \gamma + L_{yx} \bar{C}_f^2 \alpha^2 \right) (1 - \beta \mu_g)^S \mathbb{E}[\| y^k - y^*(x^k) \|^2]
\]

\[
+ \left( 1 + \gamma + L_{yx} \bar{C}_f^2 \alpha^2 \beta \sqrt{\sigma_{g,1}^2 + (L_y^2 + L_{yx}) \alpha^2 \sigma_{f}^2} \right) + \left( L_y^2 + L_{yx} + \frac{L_y^2}{\gamma} \right) \alpha^2 \mathbb{E} \left[ \| \bar{h}_k \|_{P_x}^2 \right].
\]

We can define Lyapunov function as

\[
\gamma^k := F(x^k) + \frac{L_f}{L_y} \| y^*(x^k) - y^k \|^2.
\]

Using Lemma 12–14, we get

\[
\mathbb{E} \left[ \gamma^{k+1} \right] - \mathbb{E} \left[ \gamma^k \right] \leq -\alpha \frac{\mathbb{E} \left[ \| \nabla F(x^k) \|_{P_x}^2 \right]}{2} + \alpha L_f^2 (1 - \beta \mu_g)^S \mathbb{E} \left[ \| y^k - y^*(x^k) \|^2 \right] + \alpha h_k^2
\]

\[
- \left( \frac{\alpha}{2} \frac{L_f \alpha^2}{2} \right) \mathbb{E} \left[ \| \bar{h}_k \|_{P_x}^2 \right] + \frac{L_f \alpha^2 \sigma_{f}^2}{2}.
\]
Since we also need to

Denoting \( \alpha \leq \min \left( \frac{1}{2L_F + 4L_f L_y + \frac{4L_f L_y}{L_y}}, \frac{\mu_g}{\ell_{g,1}(5L_f L_y + L_y \hat{C}_f^2)} \right) \),

Choosing \( \alpha \leq 1 \), the sufficient condition of making the last two terms in (74) negative becomes

\[
\alpha \leq \min \left( \frac{1}{2L_F + 4L_f L_y + \frac{4L_f L_y}{L_y}}, \frac{\mu_g}{\ell_{g,1}(5L_f L_y + L_y \hat{C}_f^2)} \right),
\]

Since we also need \( \beta \leq \frac{1}{\ell_{g,1}} \), then the sufficient condition for (75) becomes

\[
\alpha \leq \min \left( \frac{1}{2L_F + 4L_f L_y + \frac{4L_f L_y}{L_y}}, \frac{\mu_g}{\ell_{g,1}(5L_f L_y + L_y \hat{C}_f^2)} \right), \quad \beta = \frac{5L_f L_y + L_y \hat{C}_f^2}{\mu_g} \alpha.
\]

Denoting

\[
\tilde{\alpha}_1 = \frac{1}{2L_F + 4L_f L_y + \frac{4L_f L_y}{L_y}}, \quad \tilde{\alpha}_2 = \frac{\mu_g}{\ell_{g,1}(5L_f L_y + L_y \hat{C}_f^2)}
\]

and choosing \( \alpha = \min \left( \tilde{\alpha}_1, \tilde{\alpha}_2, \frac{\mu_g}{\sqrt{2}} \right) \), then (74) becomes

\[
\frac{\alpha}{2} \mathbb{E}[\|\nabla F(x^k)\|_{P_{\gamma}}^2] \leq \left( \mathbb{E}[\mathbb{V}_0^k] - \mathbb{E}[\mathbb{V}_{k+1}] \right) + c_1 S \alpha_2^2 \sigma_{g,1}^2 + c_2 \alpha_2^2 \hat{\sigma}_f^2 + \alpha b_k^2.
\]
where \( c_1 \) and \( c_2 \) are defined as
\[
c_1 = \frac{L_f}{L_y} \left( 1 + 5L_f L_y \alpha + L_yx \tilde{C}_f^2 \alpha^2 \right) \left( \frac{5L_f L_y + L_yx \tilde{C}_f^2 \alpha^2}{\mu_y \beta} \right)^2
\]
\[
c_2 = \frac{L_F}{2} + \frac{L_f}{L_y} \left( L_y^2 + L_yx \right).
\]

Telescoping (76) and dividing both sides by \( \frac{1}{4} \sum_{k=0}^{K-1} \alpha \) leads to
\[
\frac{1}{K} \sum_{k=0}^{K-1} \alpha \mathbb{E} \left[ \left\| \nabla F(x^k) \right\|_{P_x}^2 \right] \leq \frac{\mathbb{E} \left[ \sum_{k=0}^{K-1} (\alpha b_k^2 + c_1 S \sigma^2_{g,1} + c_2 \alpha \hat{\sigma}_f^2) \right]}{\frac{1}{2} \sum_{k=0}^{K-1} \alpha K} = \tilde{O} \left( \frac{1}{\sqrt{K}} \right).
\]

We then let \( \tilde{\alpha}, S = \mathcal{O}(1) \) and \( N = \mathcal{O}(\log K) \) so that \( b_k^2 \leq \mathcal{O}(1/\sqrt{K}) \) and \( \hat{\sigma}_f^2 = \mathcal{O}(N) = \mathcal{O}(\log K) \), and thus,
\[
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \left\| \nabla F(x^k) \right\|_{P_x}^2 \right] \leq \mathbb{E} \left[ \sum_{k=0}^{K-1} (\alpha b_k^2 + c_1 S \sigma^2_{g,1} + c_2 \alpha \hat{\sigma}_f^2) \right] = \tilde{O} \left( \frac{1}{\sqrt{K}} \right).
\]

This implies that Algorithm 1 achieves an \( \epsilon \)-stationary point by \( K = \tilde{O}(\epsilon^{-2}) \) iterations. \( \blacksquare \)

### C Theoretical Analysis for E-AiPOD

In this section, we present the proof of Algorithm 2. We define
\[
\tilde{\mathcal{X}}_k := \sigma \{ y^0, x^0, \ldots, y^{k+1}, x^{k+1}, \ldots, x^{k,t} \} \tag{77}
\]
where \( \sigma \{ \cdot \} \) denotes the \( \sigma \)-algebra generated by the random variables. Then it follows that \( \tilde{\mathcal{X}}_k = \sigma \{ y^0, x^0, \ldots, y^{k+1} \} \).

#### C.1 Descent of upper level

First, we notice that the update of E-AiPOD in (12) can be written as
\[
x^{k+1} \overset{(a)}{=} (1 - \delta)x^k + \delta \text{Proj}_{\mathcal{X}} \left( x^k - \alpha \sum_{t=0}^{T-1} h^{k,t}_f \right)
\]
\[
\overset{(b)}{=} (1 - \delta)x^k + \delta (I - B^\dagger B) \left( x^k - \alpha \sum_{t=0}^{T-1} h^{k,t}_f \right) + \delta B^\dagger e
\]
\[
= (1 - \delta)x^k + \delta \text{Proj}_{\mathcal{X}}(x^k) - \alpha \delta \sum_{t=0}^{T-1} (I - B^\dagger B)h^{k,t}_f
\]
\[
\overset{(c)}{=} x^k - \alpha \delta (I - B^\dagger B) \left( \sum_{t=0}^{T-1} h^{k,t}_f \right)
\]
where \( (a) \) comes from the update rule in (11a) and (12), \( (b) \) is derived from the closed form of \( \text{Proj}(\cdot) \) on the linear space \( \mathcal{X} = \{ x \mid Bx = e \} \), and \( (c) \) holds since \( x^k \in \mathcal{X} \).

We first quantify the bias induced by using the Hessian inverse vector product at a different point.
Lemma 15 (Error of using delayed Hessian vector product). Define
\[ G(x, y, \tilde{x}) := \nabla_x f(x, y) + \left[ \left( \nabla h(\tilde{x})^T A^T \nabla_y g(\tilde{x}, y) - \nabla xy g(\tilde{x}, y) \right) \times V_2 (V_2^T \nabla_y g(\tilde{x}, y)V_2)^{-1}V_2^T - \nabla h(\tilde{x})^T A^T \right] \nabla_y f(\tilde{x}, y) \]
as the gradient estimator using Hessian vector product at point \( \tilde{x} \). We have
\[ \| G(x, y, \tilde{x}) \| \leq \ell_{f,0}(1 + L_y) \\
\| G(x, y, \tilde{x}) - \nabla f(x, y) \| \leq L_G \| x - \tilde{x} \| \]
where \( L_G := \frac{(1+\ell_{h,0}\|A^\dagger\|)\ell_{g,1}}{\mu_g} \left( \ell_{f,1} + \frac{\ell_{f,0}\ell_{g,2}}{\mu_g} + \frac{\mu_g\ell_{g,2}}{\ell_{g,1}} \right) + (\ell_{h,0}\ell_{f,1} + \ell_{h,1}(\ell_{g,1} + \ell_{f,0})) \| A^\dagger \|. \]

**Proof:** First, since \( G(x, y, \tilde{x}) \) only differs from \( \nabla f(x, y) \) at the evaluation point \( \tilde{x} \) of Hessian vector product, the bound for \( \| G(x, y, \tilde{x}) \| \) can derive the same way as \( \nabla f(x, y) \) following Lemma 8, that is
\[ \| G(x, y, \tilde{x}) \| \leq \ell_{f,0}(1 + L_y). \]

Next, for any \( x, y, \tilde{x} \), we have that
\[ \| G(x, y, \tilde{x}) - \nabla f(x, y) \|
\leq \| \left( \nabla h(\tilde{x})^T A^T \nabla yy g(\tilde{x}, y) - \nabla xy g(\tilde{x}, y) \right) V_2 (V_2^T \nabla yy g(\tilde{x}, y)V_2)^{-1}V_2^T \nabla y f(\tilde{x}, y) \\
- \left( \nabla h(x)^T A^T \nabla yy g(x, y) - \nabla xy g(x, y) \right) V_2 (V_2^T \nabla yy g(x, y)V_2)^{-1}V_2^T \nabla y f(x, y) \|
- \| \nabla h(\tilde{x})^T A^T \nabla yy g(\tilde{x}, y) - \nabla h(x)^T A^T \nabla y f(\tilde{x}, y) \|
- \| \nabla h(\tilde{x})^T A^T \nabla yy g(\tilde{x}, y) - \nabla h(x)^T A^T \nabla y f(x, y) \|
\leq \| \nabla h(x)^T A^T \nabla yy g(x, y) - \nabla xy g(x, y) \|
\times \| V_2 (V_2^T \nabla yy g(\tilde{x}, y)V_2)^{-1}V_2^T \nabla y f(\tilde{x}, y) - V_2 (V_2^T \nabla yy g(x, y)V_2)^{-1}V_2^T \nabla y f(x, y) \|
- \| \nabla h(\tilde{x})^T A^T \nabla xy g(\tilde{x}, y) - \nabla h(x)^T A^T \nabla xy g(x, y) \|
\leq \ell_{g,1} (1 + \ell_{h,0}\|A^\dagger\|) \left( \| V_2 (V_2^T \nabla yy g(\tilde{x}, y)V_2)^{-1}V_2^T \| \| \nabla y f(\tilde{x}, y) - \nabla y f(x, y) \| \\
+ \| \nabla y f(x, y) \| \| V_2 ((V_2^T \nabla yy g(\tilde{x}, y)V_2)^{-1} - (V_2^T \nabla yy g(x, y)V_2)^{-1}) V_2^T \| \right) \\
+ \| \nabla xy g(\tilde{x}, y) - \nabla xy g(x, y) \| + \| \nabla h(\tilde{x})^T A^T \nabla yy g(\tilde{x}, y) - \nabla h(x)^T A^T \nabla yy g(x, y) \|
+ \ell_{h,0}\ell_{f,1}\|A^\dagger\|\| \tilde{x} - x \| + \ell_{h,1}\ell_{f,0}\|A^\dagger\|\| x - \tilde{x} \|
\leq \frac{(1 + \ell_{h,0}\|A^\dagger\|)\ell_{g,1}}{\mu_g} \left( \ell_{f,1} + \frac{\ell_{f,0}\ell_{g,2}}{\mu_g} + \frac{\mu_g\ell_{g,2}}{\ell_{g,1}} \right) + (\ell_{h,0}\ell_{f,1} + \ell_{h,1}(\ell_{g,1} + \ell_{f,0})) \| A^\dagger \| \| x - \tilde{x} \| \]
where (a) and (b) hold similarly with the derivation of (38).

Lemma 15 shows the bias induced by evaluating the Hessian inverse vector product at a different point can be controlled by the point difference. We have the counterpart of Lemma 12 as below.
Lemma 16 (Bias and variance of gradient estimator). Let \( \tilde{c} = \frac{\mu_g}{\mu_g^2 + \sigma_g^2} \) and define

\[
\tilde{h}^{k,t} := \mathbb{E}[h^{k,t} | \mathcal{F}^0_k],
\]

then \( \tilde{h}^{k,t}_f \) is a biased estimator of upper-level gradient which satisfies that

\[
\mathbb{E} \left[ \left\| \frac{1}{T} \sum_{t=0}^{T-1} (h^{k,t}_f - \tilde{h}^{k,t}_f) \right\|^2 \right] \leq \frac{\sigma_f^2}{T}, \tag{80}
\]

Proof: We omit the proof of (79) since it is almost the same as the proof of Lemma 12, and only prove (80). For (80), we have

\[
\mathbb{E} \left[ \left\| \frac{1}{T} \sum_{t=0}^{T-1} (h^{k,t}_f - \tilde{h}^{k,t}_f) \right\|^2 \right] \leq \frac{1}{T^2} \mathbb{E} \left[ \left\| \sum_{t=0}^{T-1} h^{k,t}_f - \tilde{h}^{k,t}_f \right\|^2 \right] \mathbb{E} \left[ \left\| \mathcal{F}^{T-1}_k \right\| \right] \mathbb{E} \left[ \left\| \mathcal{F}_k^0 \right\| \right] \tag{a}
\]

\[
= \frac{1}{T^2} \mathbb{E} \left[ \left\| h^{k,T-1}_f - \tilde{h}^{k,T-1}_f \right\|^2 \right] + \frac{1}{T^2} \mathbb{E} \left[ \left\| \sum_{t=0}^{T-2} h^{k,t}_f - \tilde{h}^{k,t}_f \right\|^2 \right] \mathbb{E} \left[ \left\| \mathcal{F}_k^0 \right\| \right] \tag{b}
\]

where (a) holds since \( h^{k,T-1}_f - \tilde{h}^{k,T-1}_f \) is independent from \( \sum_{t=0}^{T-2} h^{k,t}_f - \tilde{h}^{k,t}_f \) when given \( \mathcal{F}^*_k,T-1 \); and (b) follows from applying the previous procedure \( T - 1 \) times. \( \blacksquare \)

We then state a lemma controlling the drifting error of lazy projections.

Lemma 17 (Drifting error of upper level). Under Assumption 1–4, it holds that for any \( t \),

\[
\mathbb{E} \left[ \left\| x^{k,t} - x^k \right\|^2 \right] \leq \alpha^2 t^2 \tilde{C}^2_f
\]

where \( \tilde{C}^2_f = 2\bar{v}^2_t + 2\ell^2_{f,0} (1 + L_y)^2 + \tilde{\sigma}_f^2 \).

Proof: For any \( t \), we know that

\[
\mathbb{E} \left[ \left\| x^{k,t+1} - x^{k,t} \right\|^2 \right] = \mathbb{E} \left[ \left\| x^{k,t+1} - x^{k,t} \right\|^2 \right] = \mathbb{E} \left[ \left\| x^{k,t} - \alpha h^{k,t}_f - x^{k,t} \right\|^2 \right] = \alpha^2 \mathbb{E} \left[ \left\| h^{k,t}_f \right\|^2 \right] \tag{a} \leq \alpha^2 \tilde{C}^2_f
\]

(81)
where (a) is derived similarly from the bound for $\mathbb{E}[\|h^k_f\|^2]$ in (70) based on Lemma 15 and Lemma 16 and the constant is defined as $\bar{C}^2_f = 2\beta^2 + 2\sigma^2_f + \alpha^2_f$.

Then for any $t$, it holds that
\[
\mathbb{E} \left[ \|x^{k,t} - x^k\|^2 \right] = \mathbb{E} \left[ \|x^{k,t} - x^{k,t-1} + x^{k,t-1} - x^{k,t-2} + \cdots - x^k\|^2 \right] \\
\leq t \sum_{\tau=0}^{t-1} \mathbb{E} \left[ \|x^{k,\tau+1} - x^{k,\tau}\|^2 \right] \leq \alpha^2 t^2 \bar{C}^2_f
\]
which completes the proof.

**Lemma 18.** Under Assumption 1–4 and let $N = O(\log \alpha^{-1})$, it holds that
\[
\mathbb{E} \left[ \left\| \frac{1}{T} \sum_{t=0}^{T-1} \bar{h}^{k,t}_f - \nabla f(x^k, y^{k+1}) \right\|^2 \right] = O(\alpha^2 T^2). \tag{82}
\]

**Proof:** For any $t$, we have that
\[
\mathbb{E} \left[ \|\bar{h}^{k,t}_f - \nabla f(x^k, y^{k+1})\|^2 \right] \leq 3\mathbb{E}[\|\bar{h}^{k,t}_f - G(x^{k,t}, y^{k+1}, x^k)\|^2] + 3\mathbb{E}[\|\nabla f(x^{k,t}, y^{k+1}) - \nabla f(x^k, y^{k+1})\|^2] \\
+ 3\mathbb{E}[\|G(x^{k,t}, y^{k+1}, x^k) - \nabla f(x^{k,t}, y^{k+1})\|^2] \\
\leq (a) 3\beta^2_k + 3L^2_G\mathbb{E}[\|x^{k,t} - x^k\|^2] + 3L^2_f\mathbb{E}[\|x^{k,t} - x^k\|^2] \\
\leq (b) 3\beta^2_k + 3\alpha^2(L^2_G + L^2_f)\sigma^2_f \leq (c) O(\alpha^2 T^2) \tag{83}
\]
where (a) is due to Lemma 15, (b) comes from Lemma 17 and (c) holds by (51) and $N = O(\log \alpha^{-1})$.

Using the fact that $\left\| \frac{1}{T} \sum_{t=0}^{T-1} \bar{z}_t \right\|^2 = \frac{1}{T^2} \left\| \sum_{t=0}^{T-1} \bar{z}_t \right\|^2 \leq \frac{1}{T} \sum_{t=0}^{T-1} \|z_t\|^2$, from (83), we have
\[
\mathbb{E} \left[ \left\| \frac{1}{T} \sum_{t=0}^{T-1} \bar{h}^{k,t}_f - \nabla f(x^k, y^{k+1}) \right\|^2 \right] = O(\alpha^2 T^2) \tag{84}
\]
from which the proof is complete.

**Lemma 19 (Descent of upper level).** Under Assumption 1–4, if we define $\bar{H}^k_f := \frac{1}{T} \sum_{t=0}^{T-1} \bar{h}^{k,t}_f$, it holds that
\[
\mathbb{E}[F(x^{k+1})] \leq \mathbb{E}[F(x^k)] - \frac{\alpha T}{2} \mathbb{E}[\|\nabla F(x^k)\|^2] - \frac{\alpha^2 T^2}{2} \mathbb{E}[\|\bar{H}^k_f\|^2_{P_x}] + \frac{\alpha^2 L_T^2}{2} \mathbb{E}[\|\bar{H}^k_f\|^2_{P_x}] + \frac{\alpha^2 L_T^2}{2} \mathbb{E}[\|y^{k+1} - y^x(x^k)\|^2] + O(\alpha^2 T^2).
\]

**Proof:** First, we have
\[
\mathbb{E} \left[ \left\| \frac{1}{T} \sum_{t=0}^{T-1} h^{k,t}_f \right\|^2_{P_x} \right] = \mathbb{E} \left[ \left\| \frac{1}{T} \sum_{t=0}^{T-1} h^{k,t}_f - \bar{h}^{k,t}_f + \bar{h}^{k,t}_f \right\|^2_{P_x} \right]
\]
\[ \begin{align*}
&\overset{(a)}{=} \mathbb{E} \left[ \left\| \frac{1}{T} \sum_{t=0}^{T-1} h_{f,t}^{k,t} \right\|_{P_x}^2 \right] + \mathbb{E} \left[ \left\| \frac{1}{T} \sum_{t=0}^{T-1} h_{f,t}^{k,t} \right\|_{P_x}^2 \right] \\
&\overset{(b)}{\leq} \mathbb{E} \left[ \| \bar{H}_f^k \|_{P_x}^2 \right] + \frac{\sigma_f^2}{T}
\end{align*} \]

where (a) follows from Lemma 5 and (b) results from (80).

Moreover, it follows that

\[ \mathbb{E} \left[ \langle \nabla F(x^k), (I - B^\dagger B) \frac{1}{T} \sum_{t=0}^{T-1} h_{f,t}^{k,t} \rangle \right] = \mathbb{E} \left[ \frac{1}{T} \sum_{t=0}^{T-1} \mathbb{E} \left[ \langle \nabla F(x^k), (I - B^\dagger B) h_{f,t}^{k,t} \rangle | \bar{x}^t \rangle \right] \right] = \mathbb{E} \left[ \langle \nabla F(x^k), (I - B^\dagger B) \bar{H}_f^k \rangle \right]. \]

Taking the expectation of \( F(x^{k+1}) \), we get

\[ \mathbb{E} \left[ F(x^{k+1}) \right] \overset{(a)}{\leq} \mathbb{E} \left[ F(x^k) \right] + \mathbb{E} \left[ \langle \nabla F(x^k), x^{k+1} - x^k \rangle \right] + \frac{L_F}{2} \mathbb{E} \left[ \| x^{k+1} - x^k \|_2^2 \right] \\
\overset{(b)}{\leq} \mathbb{E} \left[ F(x^k) \right] - \alpha \delta T \mathbb{E} \left[ \langle \nabla F(x^k), (I - B^\dagger B) \frac{1}{T} \sum_{t=0}^{T-1} h_{f,t}^{k,t} \rangle \right] + \frac{L_F}{2} \alpha^2 T^2 \delta^2 \mathbb{E} \left[ \left\| \frac{1}{T} \sum_{t=0}^{T-1} h_{f,t}^{k,t} \right\|_{P_x}^2 \right] \\
\overset{(c)}{\leq} \mathbb{E} \left[ F(x^k) \right] - \alpha \delta T \mathbb{E} \left[ \langle \nabla F(x^k), (I - B^\dagger B) \bar{H}_f^k \rangle \right] + \frac{L_F}{2} \alpha^2 T^2 \delta^2 \mathbb{E} \left[ \| \bar{H}_f^k \|_{P_x}^2 \right] + \frac{L_F}{2} \alpha^2 T \delta^2 \sigma_f^2 \\
\overset{(d)}{\leq} \mathbb{E} \left[ F(x^k) \right] - \alpha \delta T \mathbb{E} \left[ \| \nabla F(x^k) \|_{P_x}^2 \right] - \left( \frac{\alpha \delta T}{2} - \frac{\alpha^2 L_F T^2 \delta^2}{2} \right) \mathbb{E} \left[ \| \bar{H}_f^k \|_{P_x}^2 \right] \\
+ \frac{\alpha \delta T}{2} \mathbb{E} \left[ \| \nabla F(x^k) - \bar{H}_f^k \|_2^2 \right] + \frac{\alpha^2 \delta^2 L_F T \sigma_f^2}{2} \\
\leq \mathbb{E} \left[ F(x^k) \right] - \alpha \delta T \mathbb{E} \left[ \| \nabla F(x^k) \|_{P_x}^2 \right] - \left( \frac{\alpha \delta T}{2} - \frac{\alpha^2 \delta^2 L_F T^2}{2} \right) \mathbb{E} \left[ \| \bar{H}_f^k \|_{P_x}^2 \right] + \frac{\alpha^2 \delta^2 L_F T \sigma_f^2}{2} \\
+ \alpha \delta T \mathbb{E} \left[ \| \nabla F(x^k) - \nabla f(x^k, y^{k+1}) \|_2^2 \right] + \alpha \delta T \mathbb{E} \left[ \| \nabla f(x^k, y^{k+1}) - \bar{H}_f^k \|_2^2 \right] \\
\overset{(e)}{\leq} \mathbb{E} \left[ F(x^k) \right] - \alpha \delta T \mathbb{E} \left[ \| \nabla F(x^k) \|_{P_x}^2 \right] - \left( \frac{\alpha \delta T}{2} - \frac{\alpha^2 \delta^2 L_F T^2}{2} \right) \mathbb{E} \left[ \| \bar{H}_f^k \|_{P_x}^2 \right] + \frac{\alpha^2 \delta^2 L_F T \sigma_f^2}{2} \\
+ \alpha T \delta^2 \mathbb{E} \left[ \| y^{k+1} - y^* (x^k) \|_2^2 \right] + O(\alpha^3 T^3 \delta)
\]

where (a) comes from the smoothness of \( F \) and the update (78), (b) is derived from (78), and (c) results from (85) and (86), (d) comes from \( 2a^\dagger b = \|a\|^2 + \|b\|^2 - \|a - b\|^2 \) and \( \|I - B^\dagger B\| \leq 1 \), (e) is derived from Lipschitz continuity of \( \nabla f(x, y) \), \( F(x) = \nabla f(x, y^* (x)) \) and Lemma 18. This completes the proof.
C.2 Error of lower level

Lemma 20 (Lipschitz continuity and smoothness of the \( r^*(x) \)). Under Assumption 1–2, the projection offset \( r^*(x) \) is \( L_r \)-Lipschitz continuous and \( L_{rx} \)-smooth with constants defined as

\[
L_r := \ell_{g,1}(1 + L_y), \quad \text{and} \quad L_{rx} := \ell_{g,2}(1 + L_y)^2 + \ell_{g,1}L_{yx}.
\]

Proof: Recall the definition of \( r^*(x) := \nabla y g(x, y^*(x)) \), then for any \( x_1, x_2 \),

\[
\|r^*(x_1) - r^*(x_2)\| \leq \|\nabla y g(x_1, y^*(x_1)) - \nabla y g(x_2, y^*(x_2))\|
\leq \ell_{g,1}(\|x_1 - x_2\| + \|y^*(x_1) - y^*(x_2)\|)
\leq \ell_{g,1}(1 + L_y)\|x_1 - x_2\| = L_r\|x_1 - x_2\|.
\]

Using the chain rule, we can obtain the gradient of \( r^*(x) \) as

\[
\nabla r^*(x) = \nabla_{yx} g(x, y^*(x)) + \nabla_{yy} g(x, y^*(x)) \nabla y^*(x).
\]

According to the Lipschitz continuity of \( \nabla y^*(x) \) and \( \nabla^2 g \), we get for any \( x_1, x_2 \)

\[
\|\nabla r^*(x_1) - \nabla r^*(x_2)\| \leq \|\nabla_{yx} g(x_1, y^*(x_1)) - \nabla_{yx} g(x_2, y^*(x_2))\|
+ \|\nabla_{yy} g(x_1, y^*(x_1)) \nabla y^*(x_1) - \nabla_{yy} g(x_2, y^*(x_2)) \nabla y^*(x_2)\|
\leq \ell_{g,2}(1 + L_y)\|x_1 - x_2\| + \|\nabla_{yy} g(x_1, y^*(x_1))\||\|\nabla y^*(x_1) - \nabla y^*(x_2)\|
\leq \ell_{g,2}(1 + L_y)\|x_1 - x_2\| + \ell_{g,1}L_{yx}\|x_1 - x_2\| = L_{rx}\|x_1 - x_2\|
\]

where (a) is derived from (40) and Lemma 3.

Lemma 21 (Error of lower-level update). Suppose that Assumption 1–4 hold and \( \beta \leq \frac{1}{\ell_{g,1}} \), then the error of lower-level update can be bounded by

\[
\mathbb{E}\left[\|y^{k+1} - y^*(x^k)\|^2 + \frac{\beta^2}{\rho^2}\|r^{k+1} - r^*(x^k)\|^2\right]
\leq (1 - \nu)^S \mathbb{E}\left[\|y^k - y^*(x^k)\|^2 + \frac{\beta^2}{\rho^2}\|r^k - r^*(x^k)\|^2\right] + S\beta^2\sigma_{g,1}^2
\]

\[
\mathbb{E}[\|y^{k+1} - y^*(x^{k+1})\|^2] \leq (1 + \gamma + 2L_{yx}C^2_{\delta}T^2\alpha^2\delta^2) \mathbb{E}[\|y^k - y^*(x^k)\|^2]
+ \left(L_y^2 + L_{yx}\right)\alpha^2\delta^2T\hat{\delta}^2 + \left(L_y^2 + L_{yx} + \frac{L_y^2}{\gamma}\right)\alpha^2\delta^2T^2\mathbb{E}\left[\|\vec{H}_\delta\|^2\|p\|^2\right]
\]

\[
\mathbb{E}[\|r^{k+1} - r^*(x^{k+1})\|^2] \leq (1 + \gamma + 2L_{rx}C^2_{\delta}T^2\alpha^2\delta^2) \mathbb{E}[\|r^k - r^*(x^k)\|^2]
+ \left(L_r^2 + L_{rx}\right)\alpha^2\delta^2T\hat{\delta}^2 + \left(L_r^2 + L_{rx} + \frac{L_r^2}{\gamma}\right)\alpha^2\delta^2T^2\mathbb{E}\left[\|\vec{H}_\delta\|^2\|p\|^2\right]
\]

where \( C^2_{\delta} \) is defined in Lemma 14, \( \nu := \min\{\beta\mu_y, \rho^2\} \), \( \gamma \) is the balancing parameter that will be chosen in the final theorem.
Proof: First, for a given $x^k$, defining $\nu := \min \left( \beta \mu_g, \rho^2 \right)$ and applying Lemma C.1 and Lemma C.2 in [50], we can obtain that

$$
\mathbb{E} \left[ \|y^{k,s+1} - y^*(x^k)\|_2^2 + \frac{\beta^2}{\rho^2} \|r^{k,s+1} - r^*(x^k)\|_2^2 \mid \mathcal{F}_{k,s} \right] 
\leq (1 - \nu) \left[ \|y^{k,s} - y^*(x^k)\|_2^2 + \frac{\beta^2}{\rho^2} \|r^{k,s} - r^*(x^k)\|_2^2 \right] + \beta^2 \sigma^2_{g,1}.
$$

(88)

Then taking the expectation of the both sides of (88) and telescoping it, we can arrive at (87a).

Next, proof of (87b) and (87c) are similar with only difference on Lipschitz constant, so that we only prove (87c). For (87c), we have

$$
\|r^{k+1} - r^*(x^{k+1})\|^2 = \underbrace{\|r^{k+1} - r^*(x^k)\|^2 + \|r^*(x^k) - r^*(x^{k+1})\|^2}_{J_1}
+ 2 \underbrace{\langle r^{k+1} - r^*(x^k), r^*(x^k) - r^*(x^{k+1}) \rangle}_{J_2}.
$$

Since $r^*(x)$ is $L_r$ Lipschitz continuous according to Lemma 20, $J_1$ can be bounded by

$$
\mathbb{E} [J_1] \leq L_r^2 \mathbb{E} \left[ \|x^{k+1} - x^k\|^2 \right] \overset{(a)}{=} \alpha^2 \delta^2 L_r^2 \mathbb{E} \left[ \| \sum_{t=0}^{T-1} h^k_{f,t} \|_{F_s}^2 \right]
\overset{(b)}{=} \alpha^2 \delta^2 L_r^2 \left( T^2 \mathbb{E} \left[ \| \bar{H}^k_f \|_{F_s}^2 \right] + T \bar{\sigma}^2_f \right)
$$

(89)

where (a) comes from (60), (b) is attained by (85).

On the other hand, we can decompose $J_2$ by two terms as follows.

$$
J_2 = -\langle r^{k+1} - r^*(x^k), \nabla r^*(x^k)^\top (x^{k+1} - x^k) \rangle
- \langle r^{k+1} - r^*(x^k), r^*(x^{k+1}) - r^*(x^k) - \nabla r^*(x^k)^\top (x^{k+1} - x^k) \rangle.
$$

Moreover, the conditional expectation of $J_{2,1}$ can be bounded by

$$
\mathbb{E} [J_{2,1}] = -\mathbb{E} [\langle r^{k+1} - r^*(x^k), \nabla r^*(x^k)^\top (x^{k+1} - x^k) \rangle]
= -\alpha \delta \mathbb{E} [\langle r^{k+1} - r^*(x^k), \nabla r^*(x^k)^\top (I - B^\dagger B) (\sum_{t=0}^{T-1} h^k_{f,t}) \rangle]
= -\alpha \delta \mathbb{E} \left[ \sum_{t=0}^{T-1} \mathbb{E} [\langle r^{k+1} - r^*(x^k), \nabla r^*(x^k)^\top (I - B^\dagger B) h^k_{f,t} \rangle | \mathcal{F}_k] \right]
\leq -\alpha \delta T \mathbb{E} [\langle r^{k+1} - r^*(x^k), \nabla r^*(x^k)^\top (I - B^\dagger B) \bar{H}^k_f \rangle]
\overset{(a)}{=} \frac{\gamma}{2} \mathbb{E} [\|r^{k+1} - r^*(x^k)\|^2] + \frac{\alpha^2 \delta^2 T^2 L_r^2}{\gamma} \mathbb{E} [\| \bar{H}^k_f \|_{F_s}^2].
$$

(90)

Based on the smoothness of $r^*(x)$ in Lemma 20 and Young’s inequality, $J_{2,2}$ can be bounded by

$$
\mathbb{E} [J_{2,2}] \leq \mathbb{E} \left[ \|r^{k+1} - r^*(x^k)\| \|r^*(x^{k+1}) - r^*(x^k) - \nabla r^*(x^k)^\top (x^{k+1} - x^k)\|_2^2 \right]
$$

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where (a) comes from

\[
\mathbb{E}[\|h_{f,t}^{k}\|_2^2 | \bar{F}_k] \leq 2\mathbb{E}[\|h_{f,t}^{k} - G(x^{k,t}, y^{k+1}, x^{k})\|_2^2 | \bar{F}_k] + 2\mathbb{E}[\|G(x^{k,t}, y^{k+1}, x^{k})\|_2^2 | \bar{F}_k] \\
\leq 2b_k^2 + 2\beta^2 f,l_0(1 + L_y)^2
\]

and \(\bar{C}_f^2 = 2b_k^2 + 2\beta^2 f,l_0(1 + L_y)^2 + \delta_f^2\). Then combining (89), (90) and (91), we get

\[
\mathbb{E}[\|r^{k+1} - r^*(x^{k+1})\|_2^2] \leq \left(1 + \gamma + 2L_{rx}\bar{C}_f^2T^2\alpha^2\delta_f^2\right) \mathbb{E}[\|r^{k+1} - r^*(x^{k})\|_2^2] + \left(L^2_r + L_{rx}\right) \alpha^2\delta^2T\delta_f^2 \\
+ \left(L^2_r + L_{rx} + \frac{L^2_r}{\gamma}\right) \alpha^2\delta^2T^2\mathbb{E}[\|\bar{H}_f\|_2^2 | p_z] 
\]

which completes the proof for (87c). With similar proof for (87c), we can prove (87b). \[\blacksquare\]

### C.3 Proof of Theorem 2

**Proof:** First, without loss of generality, we can assume that \(l_{g,1} \geq 1\) so that \(L_r \geq L_y, L_{rx} \geq L_{yx}\) and plugging (87b), (87c) into (87a) in Lemma 21, we get that

\[
\mathbb{E}\left[\|y^{k+1} - y^*(x^{k+1})\|^2 + \frac{\beta^2}{p^2}\|r^{k+1} - r^*(x^{k+1})\|^2\right] \\
\leq \left(1 + \gamma + 2L_{rx}\bar{C}_f^2T^2\alpha^2\delta_f^2\right) \left(1 - \nu^S\right) \mathbb{E}\left[\|y^k - y^*(x^k)\|^2 + \frac{\beta^2}{p^2}\|r^k - r^*(x^k)\|^2\right] \\
+ \left(1 + \gamma + 2L_{rx}\bar{C}_f^2\alpha^2\delta^2T^2\right) \left(1 + \frac{\beta^2}{p^2}\right) \alpha^2\delta^2T\delta_f^2 \\
+ \left(L^2_r + L_{rx} + \frac{L^2_r}{\gamma}\right) \left(1 + \frac{\beta^2}{p^2}\right) \alpha^2\delta^2T^2\mathbb{E}[\|\bar{H}_f\|_2^2 | p_z]. \tag{92}
\]

Then using Lyapunov function defined in (13) and applying (92), Lemma 19 and Lemma 21, we get

\[
\mathbb{E}\left[\psi_{1}^{k+1}\right] - \mathbb{E}\left[\psi_{1}^{k}\right]
\]
\[
\begin{align*}
&\leq -\frac{\alpha\delta T}{2} \mathbb{E}\left[\|\nabla F(x^k)\|_F^2\right] + \alpha\delta TL_f^2 \mathbb{E}\left[\|y^{k+1} - y^*(x^k)\|^2\right] + O(\alpha^3 T^3 \delta) \\
&\quad - \left(\frac{\alpha\delta T}{2} - \frac{L_F\alpha^2\delta^2 T^2}{2}\right) \mathbb{E}\left[\|\tilde{H}_f^k\|_{P_x}^2\right] + \frac{L_{f}}{L_r} \left(1 + \gamma + 2L_{rx}\tilde{C}_f^2\alpha^2\delta^2 T^2\right) (1 - \nu)^S - 1 \mathbb{E}\left[\|y^k - y^*(x^k)\|^2 + \frac{\beta^2}{\mu_p^2}\|r^k - r^*(x^k)\|^2\right] \\
&\quad + \frac{L_{f}}{L_r} \left(1 + \gamma + 2L_{rx}\tilde{C}_f^2\alpha^2\delta^2 T^2\right) S\beta^2\sigma_{g,1}^2 + \frac{L_{f}}{L_r} \left( L_r^2 + L_{rx} \right) \left(1 + \frac{\beta^2}{\mu_p^2}\right) \alpha^2\delta^2 T^2 \hat{\sigma}_f^2 \\
&\quad + \frac{L_{f}}{L_r} \left( L_r^2 + L_{rx} \right) \left(1 + \frac{\beta^2}{\mu_p^2}\right) \alpha^2\delta^2 T^2 \mathbb{E}\left[\|\tilde{H}_f^k\|_{P_x}^2\right] \\
&\leq -\frac{\alpha\delta T}{2} \mathbb{E}\left[\|\nabla F(x^k)\|_F^2\right] + \frac{L_{f}}{L_r} \left(1 + \gamma + L_r L_f\alpha\delta T + 2L_{rx}\tilde{C}_f^2\alpha^2\delta^2 T^2\right) \beta^2\sigma_{g,1}^2 + O(\alpha^3 T^3 \delta) \\
&\quad + \left[\frac{L_F}{2} + \frac{L_f}{L_r} \left( L_r^2 + L_{rx} \right) \left(1 + \frac{\beta^2}{\mu_p^2}\right)\right] \alpha^2\delta^2 T^2 \hat{\sigma}_f^2 \\
&\quad - \left[\frac{\alpha\delta T}{2} - \left(\frac{L_F}{2} + L_f L_r \left(1 + \frac{1}{\gamma}\right) \left(1 + \frac{\beta^2}{\mu_p^2}\right) + \frac{L_f L_{rx}}{L_r} \left(1 + \frac{\beta^2}{\mu_p^2}\right)\right) \alpha^2\delta^2 T^2 \right] \mathbb{E}\left[\|\tilde{H}_f^k\|_{P_x}^2\right] \\
&\quad - \left(\frac{L_f \mu_g \beta}{L_r} - 5\alpha\delta L_f^2 T - \frac{2L_L L_{rx}\tilde{C}_f^2\alpha^2\delta^2 T^2}{L_r}\right) \mathbb{E}\left[\|y^k - y^*(x^k)\|^2 + \frac{\beta^2}{\mu_p^2}\|r^k - r^*(x^k)\|^2\right].
\end{align*}
\]

Selecting \( \gamma = 4L_f L_r \alpha\delta T, p = \sqrt{\beta \mu_g} \), (93) can be simplified by

\[
\begin{align*}
&\mathbb{E}[V_{k+1}^1] - \mathbb{E}[V_1^1] \\
&\leq -\frac{\alpha\delta T}{2} \mathbb{E}\left[\|\nabla F(x^k)\|_F^2\right] + \frac{L_{f}}{L_r} \left(1 + 5L_f L_r\alpha\delta T + 2L_{rx}\tilde{C}_f^2\alpha^2\delta^2 T^2\right) \beta^2\sigma_{g,1}^2 + O(\alpha^3 T^3 \delta) \\
&\quad + \left[\frac{L_F}{2} + \frac{L_f}{L_r} \left( L_r^2 + L_{rx} \right) \left(1 + \frac{\beta}{\mu_g}\right)\right] \alpha^2\delta^2 T^2 \hat{\sigma}_f^2 \\
&\quad - \left[\frac{\alpha\delta T}{4} - \left(\frac{L_F}{2} + L_f L_r + \frac{L_f L_{rx}}{L_r} \right) \alpha^2\delta^2 T^2 - \frac{\beta \alpha\delta T}{4\mu_g} - \left( L_f L_r + \frac{L_f L_{rx}}{L_r} \right) \frac{\beta \alpha^2\delta^2 T^2}{\mu_g}\right] \mathbb{E}\left[\|\tilde{H}_f^k\|_{P_x}^2\right] \\
&\quad - \left(\frac{L_f \mu_g \beta}{L_r} - 5\alpha\delta L_f^2 T - \frac{2L_f L_{rx}\tilde{C}_f^2\alpha^2\delta^2 T^2}{L_r}\right) \mathbb{E}\left[\|y^k - y^*(x^k)\|^2 + \frac{\beta^2}{\mu_p^2}\|r^k - r^*(x^k)\|^2\right].
\end{align*}
\]

Let \( \alpha\delta T \leq 1 \). Since we also need \( \beta \leq \frac{1}{\mu_{g,1}} \), the sufficient condition of making the last two terms in (94) negative becomes

\[
\alpha\delta \leq \frac{\tilde{\alpha}}{T}, \quad \beta = \frac{5L_f L_r + 2L_{rx}\tilde{C}_f^2}{\mu_g} \alpha\delta \tilde{T}
\]

where \( \tilde{\alpha} = \min(\tilde{\alpha}_1, \tilde{\alpha}_2) \) and \( \tilde{\alpha}_1, \tilde{\alpha}_2 \) are defined as

\[
\tilde{\alpha}_1 = \frac{1}{2L_F + 4\mu_g L_r + \frac{4L_f L_{rx}}{L_r} + \frac{(5L_f L_r + L_{rx})}{\mu_g} \left(1 + 4L_f L_r + \frac{4L_f L_{rx}}{L_r}\right)}, \quad \tilde{\alpha}_2 = \frac{\mu_g}{\ell_{g,1}(5L_f L_r + L_{rx}\tilde{C}_f)}.
\]

(95)
According to the optimality condition, we know that

\[
\tilde{\sigma} = \sigma_c
\]

where \( \sigma_c \) is defined as

\[
\sigma_c \triangleq c_1 S \alpha^2 \delta^2 T^2 \sigma_g^2 + c_2 \alpha^2 \delta^2 T \tilde{\sigma}_f^2 + O(\alpha^3 \delta^3 T^2)
\]

where \( c_1 \) and \( c_2 \) are defined as

\[
c_1 = \frac{L_f S}{L_r} \left( 1 + L_{rx} \bar{C}_f \alpha^2 \right)^2 \left( \frac{5L_f L_r + 2L_{rx} \bar{C}_f^2}{\mu_g} \right) \quad \text{and} \quad c_2 = \frac{L_F}{2} + \frac{L_f}{L_r} \left( L_r^2 + L_{rx} \right)
\]

Telescoping (96) and dividing both sides by \( \alpha \delta T K \) leads to

\[
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E} \left[ \| \nabla F(x^k) \|_{\mathcal{F}_k}^2 \right] \leq \frac{2(\mathbb{E}[V_1^0] - F^\star)}{\alpha \delta T K} + 2c_1 \sigma_c^2 \alpha \delta T + 2c_2 \sigma_f^2 \alpha \delta + O(\alpha^2 \delta^2 T).
\]

This completes the proof.

\[\square\]

### D Theoretical Analysis for E2-AiPOD

This section presents the proof of E2-AiPOD. Since we introduce a new sequence \( u^k \), we define

\[
\mathcal{F}_k^n := \sigma \{ y^0, u^0, x^0, \ldots, y^{k+1}, u^{k+1}, \ldots, u^{k,n} \}
\]

where \( \sigma \{ \cdot \} \) denotes the \( \sigma \)-algebra generated by the random variables. For simplicity, we also denote

\[
d_f^k := \mathbb{E}[d_f^k | \mathcal{F}_k^n] = \nabla_x f(x^k, y^{k+1}) - \nabla_{xy} g(x^k, y^{k+1}) u^{k+1}.
\]

#### D.1 Supporting lemmas of Theorem 3

First, we prove Lemma 4 which states \( u^\star(x, y) \) is the solution of a strongly convex minimization problem with linear constraints.

**Restatement of Lemma 4.** \( u^\star(x, y) \) is the minimizer of a \( \mu_g \)-strongly convex problem, i.e.

\[
u^\star(x, y) = \arg \min_{u \in \{ u | V_1^T u = 0 \}} \frac{1}{2} \| \nabla_x g(x, y) \nabla_y f(x, y) + \nabla \frac{1}{2} g(x, y) u \|^2.
\]

**Proof:** We denote the optimal solution mapping as

\[
u^\star(x, y) = \arg \min_{u \in \{ u | V_1^T u = 0 \}} \frac{1}{2} \| \nabla_x g(x, y) \nabla_y f(x, y) + \nabla \frac{1}{2} g(x, y) u \|^2.
\]

According to the optimality condition, we know that \( \tilde{u}(x, y) \) satisfies

\[
\tilde{u}(x, y) = \text{Proj}_{\{ u | V_1^T u = 0 \}} \left( \tilde{u}(x, y) - (\nabla_y f(x, y) + \nabla_{xy} g(x, y) \tilde{u}(x, y)) \right)
\]

\[
\overset{(a)}{=} (I - V_1 V_1^T) \left( \tilde{u}(x, y) - (\nabla_y f(x, y) + \nabla_{xy} g(x, y) \tilde{u}(x, y)) \right)
\]

\[
\overset{(b)}{=} \tilde{u}(x, y) - V_2 V_2^T (\nabla_y f(x, y) + \nabla_{xy} g(x, y) \tilde{u}(x, y))
\]

(98)
where (a) comes from Lemma 6 and \((V_1^T)^\dagger = V_1\), (b) is derived from \(\bar{u}(x, y) \in \{u|V_1^Tu = 0\}\) and 
\[I - V_1V_1^T = V_2V_2^T.\] According to (98), we know that 
\[V_2V_2^T (\nabla_y f(x, y) + \nabla_{yy}g(x, y)\bar{u}(x, y)) = 0.\] (99)

By the definition of \(u^*(x, y)\) in (15), we can verify it satisfies (99) since 
\[V_2V_2^T (\nabla_y f(x, y) - \nabla_{yy}g(x, y)V_2(V_2^T \nabla_{yy}g(x, y)V_2)V_2^T \nabla_y f(x, y)) = V_2 (I - V_2^T \nabla_{yy}g(x, y)V_2(V_2^T \nabla_{yy}g(x, y)V_2)^{-1}V_2^T \nabla_y f(x, y)) = V_2 (I - I) V_2^T \nabla_y f(x, y)) = 0.
\]

Then due to uniqueness of \(\bar{u}(x, y)\), we know \(u^*(x, y) = \bar{u}(x, y)\).

Next, we will prove the boundedness of \(u^*(x, y)\) and \(e^*(x, y)\) where the latter is defined as
\[e^*(x, y) := \nabla_y f(x, y) + \nabla_{yy}g(x, y)u^*(x, y).\] (100)

**Lemma 22 (Boundedness of \(u^*(x, y)\) and \(e^*(x, y)\)).** Under Assumption 1–2, for any \(x\) and \(y\), \(u^*(x, y)\) is bounded by \(\frac{\ell_{f,0}}{\mu_g}\), and \(e^*(x, y)\) is bounded by \(\ell_{f,0}(1 + \ell_{g,1}/\mu_g)\).

**Proof:** According to the definition of \(u^*(x, y)\), we have \(\|u^*(x, y)\|\) is bounded by \(\frac{\ell_{f,0}}{\mu_g}\) since 
\[\|u^*(x, y)\| \leq \|V_2(V_2^T \nabla_{yy}g(x, y))^{-1}V_2^T \nabla_y f(x, y)\| \leq \frac{\ell_{f,0}}{\mu_g}.
\]

On the other hand, since \(e^*(x, y) = \nabla_y f(x, y) + \nabla_{yy}g(x, y)u^*(x, y)\), we have \(e^*(x, y)\) is bounded 
\[\|e^*(x, y)\| \leq \|\nabla_y f(x, y)\| + \|\nabla_{yy}g(x, y)\| u^*(x, y)\| \leq \ell_{f,0}(1 + \ell_{g,1}/\mu_g)
\] 
which completes the proof.

**D.2 Error of medium level**

Unfortunately, we cannot obtain the descent lemma for \(u^k\) using the similar procedure of Lemma 21 or applying the results in [53] since \(u^*(x, y)\) is not smooth with respect to \(x\) and \(y\). Instead, we can utilize the boundedness of \(u^*(x, y)\) and \(e^*(x, y)\).

**Lemma 23.** Suppose that Assumption 1–4 hold, \(\rho \leq \min \left\{ \frac{1}{\ell_{g,1}}, \frac{\mu_g}{\sigma_g^2} \right\}\) and \(q = \sqrt{\rho \mu_g/2}\), then we have the following inequalities
\[\mathbb{E} \left[ \|u^{k+1} - u^*(x^k, y^{k+1})\|^2 \mathcal{F}^0_k \right] \leq (1 - \rho \mu_g/2)^N C_u^2 + \frac{2\rho \sigma_u^2}{\mu_g} \] (101)
where \(C_u^2 := \ell_{f,0} \left(1/\mu_g^2 + (1 + \ell_{g,1}/\mu_g)^2\right)\) and \(\sigma_u^2 := \sigma_f^2 + \frac{\sigma_g^2 \ell_{f,0}^2}{\mu_g^2}\\.\)
Where (a) comes from $\rho$ with the above variance, we can prove the one-step contraction by where (a) is derived from Lemma 5, (b) comes from Assumption 3 and (c) is due to the boundedness of $C_u$ in Lemma 22.

Proof: First, we notice that $u^*(x, y)$ is the minimizer of a $\mu_g$-strongly convex function over a linear space according to Lemma 4, which enables us to apply the convergence results of Proxskip at our medium level. Besides, the variance of gradient estimator at $u^{k,n}$ can be bounded by

$$\mathbb{E} \left[ \| \nabla_y f(x^k, y^{k+1}; \xi_n) + \nabla_{yy} g(x^k, y^{k+1}; \phi_n) u^{k,n} - \nabla_y f(x^k, y^{k+1}) - \nabla_{yy} g(x^k, y^{k+1}) u^{k,n} \|_\mathcal{F}^n \right]$$

$$\leq \mathbb{E} \left[ \| \nabla_y f(x^k, y^{k+1}; \phi_n) - \nabla_y f(x^k, y^{k+1}) \|_\mathcal{F}^n \right]$$

$$+ \mathbb{E} \left[ \| (\nabla_{yy} g(x^k, y^{k+1}; \phi_n) - \nabla_{yy} g(x^k, y^{k+1}) ) u^{k,n} \|_\mathcal{F}^n \right]$$

$$(a) \leq \mathbb{E} \left[ u^{k,n} - u^*(x^k, y^{k+1}) \right]^2 [\mathcal{F}^n_k] + 2\sigma^2 \mathbb{E} \left[ u^*(x^k, y^{k+1}) \right]^2 [\mathcal{F}^n_k]$$

$$+ (a) \leq \sigma_f^2 + 2\sigma^2 \mathbb{E} \left[ u^{k,n} - u^*(x^k, y^{k+1}) \right]^2 [\mathcal{F}^n_k] + 2\sigma^2 \mathbb{E} \left[ u^*(x^k, y^{k+1}) \right]^2 [\mathcal{F}^n_k] + \frac{2\sigma^2 \ell^2 f,0}{\mu_g^2}$$

where (a) is derived from Lemma 5, (b) comes from Assumption 3 and (c) is due to the boundedness of $u^*(x, y)$ in Lemma 22.

Then, defining $\sigma_u^2 := \sigma_f^2 + 2\sigma^2 \mathbb{E} \left[ u^{k,n} - u^*(x^k, y^{k+1}) \right]^2 [\mathcal{F}^n_k] + 2\sigma^2 \mathbb{E} \left[ u^*(x^k, y^{k+1}) \right]^2 [\mathcal{F}^n_k]$ with the above variance, we can prove the one-step contraction by

$$\mathbb{E} \left[ u^{k,n+1} - u^*(x^k, y^{k+1}) \right]^2 + \frac{\rho^2}{q^2} [\mathcal{F}^n_k]$$

$$\leq \mathbb{E} \left[ (1 - \rho u_g^2 + 2\rho^2 \sigma^2 \mathbb{E} \left[ u^{k,n} - u^*(x^k, y^{k+1}) \right]^2 + (1 - q^2) \frac{\rho^2}{q^2} [\mathcal{F}^n_k] + \rho^2 \sigma_u^2$$

$$(a) \leq \mathbb{E} \left[ (1 - \rho u_g^2 / 2) [\mathcal{F}^n_k] + \rho^2 \sigma_u^2$$

$$+ (1 - \rho u_g / 2) \mathbb{E} \left[ u^{k,n} - u^*(x^k, y^{k+1}) \right]^2 + \frac{\rho^2}{q^2} [\mathcal{F}^n_k]$$

where (a) comes from $\rho \leq \frac{\mu_g}{4\sigma^2 f,0}$ and (b) is derived from the choice of $q$.

Then telescoping (102) and since $u^{k,0} = e^{k,0} = 0$, we have

$$\mathbb{E} \left[ u^{k+1} - u^*(x^k, y^{k+1}) \right]^2 [\mathcal{F}^n_k]$$

$$\leq (1 - \rho u_g / 2)^n \mathbb{E} \left[ u^*(x^k, y^{k+1}) \right]^2 + \frac{\rho^2}{q^2} [\mathcal{F}^n_k] + \rho^2 \sigma_u^2 \sum_{n=0}^N (1 - \rho u_g / 2)^n$$

$$(a) \leq (1 - \rho u_g / 2)^n \ell^2 f,0 (1/\mu_g + 1 / \ell_g,1 / \mu_g)^2 + \frac{\rho^2 \sigma_u^2}{\rho u_g / 2}$$

where (a) is derived from the boundedness of $u^*(x, y)$ and $e^*(x, y)$, and $\rho \leq q$. Then by the definition of $C_u^2$, we obtain (101).
D.3 Descent of upper level

**Lemma 24.** Suppose that Assumption 1–4 hold and choose $N = O(1/\alpha), \rho \leq \min \left\{ \frac{1}{\ell_{g,1}}, \frac{\mu_g}{4\sigma_{g,2}} \right\}$ and $q = \sqrt{\rho \mu_g}/2$, then we can obtain the following bounds

$$
\mathbb{E}[\|d^k_j\|^2 | \mathcal{F}^0_k] \leq 2\ell_{f,0}^2 \left( 1 + \frac{2\ell_{g,1}^2}{\mu_g^2} \right) + 4\ell_{g,1}^2 \left( (1 - \rho \mu_g/2)N C_u^2 + \frac{2\rho \sigma_{u}^2}{\mu_g} \right) =: C_{f,2}^2 \tag{103a}
$$

$$
\mathbb{E}[\|d^k_j - d^k_j\|^2 | \mathcal{F}^0_k] \leq 4\sigma_u^2 + 4\sigma_{g,2}^2 \left( (1 - \rho \mu_g/2)N C_u^2 + \frac{2\rho \sigma_{u}^2}{\mu_g} \right) =: \sigma_{f,2}^2 \tag{103b}
$$

where $\sigma_u^2 := \frac{\sigma_u^2 \ell_{f,0}^2}{\mu_g^2}$.

**Proof:** For $x$-sequence, we have

$$
\|d^k_j\|^2 = \|\nabla_x f(x^k, y^{k+1}) + \nabla_{xy} g(x^k, y^{k+1})u^{k+1}\|^2 \\
\leq 2\ell_{f,0}^2 + 2\ell_{g,1}^2 \|u^{k+1}\|^2 \\
\leq 2\ell_{f,0}^2 + 4\ell_{g,1}^2 \left( \|u^{k+1} - u^*(x^k, y^{k+1})\|^2 + \|u^*(x^k, y^{k+1})\|^2 \right) \\
\leq 2\ell_{f,0}^2 + 4\ell_{g,1}^2 \left( \|u^{k+1} - u^*(x^k, y^{k+1})\|^2 + \frac{\ell_{f,0}^2}{\mu_g^2} \right) \\
= 2\ell_{f,0}^2 \left( 1 + \frac{2\ell_{g,1}^2}{\mu_g^2} \right) + 4\ell_{g,1}^2 \|u^{k+1} - u^*(x^k, y^{k+1})\|^2
$$

where the first inequality comes from Assumption 1 and the third inequality is derived from the bound for $u^*(x, y)$ in Lemma 22. Then taking expectation and using Lemma 23, we get (103a).

Also, we can bound the variance of $x$-update as

$$
\mathbb{E}[\|d^k_j - d^k_j\|^2 | \mathcal{F}^0_k] \\
= \mathbb{E} \left[ \|\nabla_x f(x^k, y^{k+1}; \xi^k) + \nabla_{xy} g(x^k, y^{k+1}; \xi^k)u^{k+1} - \nabla_x f(x^k, y^{k+1}) - \nabla_{xy} g(x^k, y^{k+1})u^{k+1}\|^2 | \mathcal{F}^0_k \right] \\
\leq 2\mathbb{E} \left[ \|\nabla_x f(x^k, y^{k+1}; \xi^k) - \nabla_x f(x^k, y^{k+1})\|^2 | \mathcal{F}^0_k \right] \\
+ 2\mathbb{E} \left[ \|\nabla_{xy} g(x^k, y^{k+1}; \xi^k) - \nabla_{xy} g(x^k, y^{k+1})\|^2 | \mathcal{F}^0_k \right] \\
\leq 2\sigma_f^2 + 2\sigma_{g,2}^2 \mathbb{E} \left[ \|u^{k+1}\|^2 | \mathcal{F}^0_k \right] \\
\leq 2\sigma_f^2 + 4\sigma_{g,2}^2 \mathbb{E} \left[ \|u^{k+1} - u^*(x^k, y^{k+1})\|^2 | \mathcal{F}^0_k \right] + 4\sigma_{g,2}^2 \mathbb{E} \left[ \|u^*(x^k, y^{k+1})\|^2 | \mathcal{F}^0_k \right] \\
\leq 2\sigma_f^2 + 4\sigma_{g,2}^2 \mathbb{E} \left[ \|u^{k+1} - u^*(x^k, y^{k+1})\|^2 | \mathcal{F}^0_k \right] + \frac{4\sigma_{g,2}^2 \ell_{f,0}^2}{\mu_g^2} \\
\leq 4\sigma_u^2 + 4\sigma_{g,2}^2 \mathbb{E} \left[ \|u^{k+1} - u^*(x^k, y^{k+1})\|^2 | \mathcal{F}^0_k \right] \\
\leq 4\sigma_u^2 + 4\sigma_{g,2}^2 \left( (1 - \rho \mu_g/2)N C_u^2 + \frac{2\rho \sigma_u^2}{\mu_g} \right)
$$
where the second inequality is from Assumption 3 and the last inequality is from Lemma 23.

The update of UL in E2-AiPOD can still be viewed as biased SGD. For simplicity, we define a virtual sequence \( \bar{x}^k := \text{Proj}_X(x^k) \). Then we have

\[
\bar{x}^{k+1} \overset{(a)}{=} \text{Proj}_X(x^k - \alpha d_f^k) \\
\overset{(b)}{=} (I - B^\dagger B)(x^k - \alpha d_f^k) + B^\dagger Be \\
= \text{Proj}_X(x^k) - \alpha(I - B^\dagger B)d_f^k \\
= \bar{x}^k - \alpha(I - B^\dagger B)d_f^k
\]

(104)

where (a) results from the update of \( x \) and (b) is derived from the definition of \( \text{Proj}(\cdot) \) on the linear space \( X = \{ x \mid Bx = e \} \). We can prove the following lemma.

**Lemma 25.** Under Assumption 1–4, if we choose \( N = O(1/\alpha) \), \( \rho \leq \min \left\{ \frac{1}{\sigma_{g,1}}, \frac{\mu_g}{4\sigma_{g,2}} \right\} \) and \( q = \sqrt{\rho \mu_g}/2 \), then the sequence of \( x^k \) generated by Algorithm 5 satisfies

\[
\mathbb{E} \left[ \| x^k - \bar{x}^k \|^2 \right] = O(\alpha^2 T^2).
\]

**Proof:** We prove this by induction. For any \( k \) s.t. \( k \mod T = 0 \), it holds that \( x^k = \bar{x}^k \). Besides, for \( (k + 1) \mod T = 0 \), we have

\[
\bar{x}^{k+1} - x^{k+1} = \bar{x}^k - \alpha(I - B^\dagger B)d_f^k - (x^k - \alpha d_f^k) \\
= \bar{x}^k - x^k + \alpha B^\dagger B d_f^k
\]

(106)

For any \( k \), let \( i(k) \leq k \) be the largest value such that \( i(k) \mod T = 0 \), then telescoping (106) and using \( \bar{x}^{i(k)} - x^{i(k)} = 0 \), we know \( \bar{x}^k - x^k = \alpha B^\dagger B \sum_{j=i(k)}^k d_f^j \). Therefore, we obtain

\[
\mathbb{E}[\| x^k - \bar{x}^k \|^2] = \mathbb{E} \left[ \left\| \alpha B^\dagger B \sum_{j=i(k)}^k d_f^j \right\|^2 \right] \overset{(a)}{\leq} \alpha^2 \mathbb{E}[\| \sum_{j=i(k)}^k d_f^j \|^2] \overset{(b)}{\leq} \alpha^2 T \sum_{j=i(k)}^k \mathbb{E}[\| d_f^j \|^2] \\
\leq \alpha^2 T \sum_{j=i(k)}^k \left\{ \mathbb{E}[\| d_f^j \|^2] + \mathbb{E}[\| d_f^j - \bar{d}_f^j \|^2] \right\} \overset{(c)}{\leq} \alpha^2 T^2 \left( C_{f,2}^2 + 4(\ell_{g,1}^2 + \sigma_{g,2}^2) \mathbb{E}[\| u^{k+1} - u^*(x^k, y^{k+1}) \|^2] + 4 \sigma_u^2 \right)
\]

(107)

where (a) holds since \( \| B^\dagger B \| \leq 1 \), (b) holds since \( \mathbb{E}[\| \sum_{i=1}^T X_i \|^2] \leq I \sum_{i=1}^T \mathbb{E}[\| X_i \|^2] \) and \( k - i(k) \leq T \), and (c) is derived from Lemma 24. Then by plugging the bound in Lemma 23 into (107) and choose \( N = O(1/\alpha) \), we obtain

\[
\mathbb{E} \left[ \| x^k - \bar{x}^k \|^2 \right] \leq \alpha^2 T^2 \left( C_{f,2}^2 + 4(\ell_{g,1}^2 + \sigma_{g,2}^2) \left( (1 - \rho \mu_g/2)^N \frac{C_u^2}{\mu_g} + \frac{2\rho \sigma_u^2}{\mu_g} \right) + 4 \sigma_u^2 \right) = O(\alpha^2 T^2)
\]

which completes the proof.  

\[\blacksquare\]
Lemma 26 (Descent of UL). Under Assumption 1–4 and setting $N = \mathcal{O}(1/\alpha)$, $\rho \leq \min\left\{\frac{1}{\ell_{g,1}}, \frac{\mu_g}{4\sigma_{\alpha,2}^2}\right\}$ and $q = \sqrt{\rho \mu_g/2}$, the virtual sequence $\bar{x}^k$ generated by Algorithm 5 satisfies

$$\mathbb{E}[F(\bar{x}^{k+1})] - \mathbb{E}[F(\bar{x}^k)] \leq -\frac{\alpha}{2} \mathbb{E}[[\nabla F(\bar{x}^k)]^2]_{P_x} - \left(\frac{\alpha}{2} - \frac{L_F \alpha^2}{2}\right) \mathbb{E}[[d_f^k]_{P_x}^2] + \frac{L_F \alpha^2 \sigma_{f,2}^2}{2} + \mathcal{O}(\alpha^3 T^2)$$

$$+ \frac{3\ell_{g,1}^2}{2}\left((1 - \rho \mu_g/2)\mathbb{E}[\parallel y^{k+1} - y^*(x^k)\parallel^2]\right)$$

where $P_x = I - B^\dagger B$ is the projection matrix of $B$ and $B^\dagger$ is the Moore-Penrose inverse of $B$.

Proof: Taking expectation given $\mathcal{F}^N_k$ and using smoothness, we obtain

$$\mathbb{E}[F(\bar{x}^{k+1})|\mathcal{F}^N_k] \leq F(\bar{x}^k) + \mathbb{E}[:\nabla F(\bar{x}^k), \bar{x}^{k+1} - \bar{x}^k:]|\mathcal{F}^N_k] + \frac{L_F}{2} \mathbb{E}[[\bar{x}^{k+1} - \bar{x}^k]_{\mathcal{F}^N_k}]$$

$$\overset{(a)}{=} F(\bar{x}^k) - \langle \nabla F(\bar{x}^k), \alpha(I-B^\dagger B)d_f^k \rangle + \frac{L_F \alpha^2}{2} \mathbb{E}[[d_f^k]_{P_x}^2|\mathcal{F}^N_k]$$

$$\overset{(b)}{=} F(\bar{x}^k) - \alpha \langle \nabla F(\bar{x}^k), (I-B^\dagger B)d_f^k \rangle + \frac{L_F \alpha^2}{2} \left\{ \mathbb{E}[[d_f^k - d_f^k]_{P_x}^2|\mathcal{F}^N_k] + \parallel d_f^k_{P_x} \parallel^2 \right\}$$

$$\overset{(c)}{=} F(\bar{x}^k) - \frac{\alpha}{2} \parallel \nabla F(\bar{x}^k) \parallel_{P_x}^2 - \left(\frac{\alpha}{2} - \frac{L_F \alpha^2}{2}\right) \parallel d_f^k_{P_x} \parallel^2$$

$$+ \frac{\alpha}{2} \parallel \nabla F(\bar{x}^k) - d_f^k \parallel^2 + \frac{L_F \alpha^2 \sigma_{f,2}^2}{2}$$

(109)

where (a) results from (104), (b) is derived from $\mathbb{E}[[X]_Y^2] = \mathbb{E}[[X]_Y]^2 + \mathbb{E}[[X - \mathbb{E}[X|Y]]_Y^2]$, and (c) holds since $2a^\top b = \parallel a \parallel^2 + \parallel b \parallel^2 - \parallel a - b \parallel^2$, $\parallel I - B^\dagger B \parallel \leq 1$ and Lemma 24.

Besides, we can decompose the bias of UL gradient estimator as

$$\parallel \nabla F(\bar{x}^k) - d_f^k \parallel^2 = \parallel \nabla F(\bar{x}^k) - \nabla f(x^k, y^{k+1}) + \nabla f(\bar{x}^k, y^{k+1}) - \nabla f(x^k, y^{k+1}) + \nabla f(x^k, y^{k+1}) - d_f^k \parallel^2$$

$$\overset{(a)}{=} 3\parallel \nabla F(\bar{x}^k) - \nabla f(x^k, y^{k+1}) \parallel^2 + 3\parallel \nabla f(\bar{x}^k, y^{k+1}) - \nabla f(x^k, y^{k+1}) \parallel^2$$

$$+ 3\parallel \nabla g(x^k, y^{k+1})u^*(x^k, y^{k+1}) - u^{k+1} \parallel^2$$

$$\overset{(b)}{=} 3L_f^2\parallel y^{k+1} - y^*(\bar{x}^k) \parallel^2 + 3L_f^2\parallel \bar{x}^k - x^k \parallel^2 + 3\ell_{g,1}^2\parallel u^{k+1} - u^*(x^k, y^{k+1}) \parallel^2$$

(110)

where (a) comes from $\parallel X + Y + Z \parallel^2 \leq 3\parallel X \parallel^2 + 3\parallel Y \parallel^2 + 3\parallel Z \parallel^2$, $\nabla F(x) = \nabla f(x, y^*)$ and $\nabla f(x, y) = \nabla_x f(x, y) + \nabla_y g(x, y)u^*(x, y)$; and (b) holds since $F(x), \nabla f(x, y)$ is Lipschitz continuous and $\nabla g(x, y)$ is bounded.

Plugging (110) into (109) and taking expectation, we get

$$\mathbb{E}[F(\bar{x}^{k+1})] \leq \mathbb{E}[F(\bar{x}^k)] - \frac{\alpha}{2} \mathbb{E}[[\nabla F(\bar{x}^k)]_{P_x}^2] - \left(\frac{\alpha}{2} - \frac{L_F \alpha^2}{2}\right) \mathbb{E}[[d_f^k]_{P_x}^2] + \frac{L_F \alpha^2 \sigma_{f,2}^2}{2}$$

$$+ \frac{3\ell_{g,1}^2}{2} \mathbb{E}[[u^{k+1} - u^*(x^k, y^{k+1})]_{P_x}^2]$$

$$+ \frac{3\alpha L_f^2}{2} \mathbb{E}[[y^{k+1} - y^*(\bar{x}^k)]_{P_x}^2] + \frac{3\alpha L_f^2}{2} \mathbb{E}[[x^k - \bar{x}^k]_{P_x}^2]$$

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\[ \leq \mathbb{E}[F(\bar{x}^k)] - \frac{\alpha}{2} \mathbb{E}[\|\nabla F(\bar{x}^k)\|^2] - \left(\frac{\alpha}{2} - \frac{L_F \alpha^2}{2}\right) \mathbb{E}[\|\bar{d}_f^k\|^2] + \frac{L_F \alpha^2 \sigma_f^2}{2} \\
+ \frac{3L^2 \alpha}{2} \left(1 - \rho \mu_g/2\right) C_u^2 + \frac{2\rho \mu_g^2}{\mu_g} \right) \mathbb{E}[\|y^{k+1} - y^*(\bar{x}^k)\|^2] + \mathcal{O}(\alpha^3 T^2) \]

where (a) results from Lemma 23 and Lemma 25. This completes the proof.

**D.4 Error of lower level**

In this section, we focus on the LL update of E2-AiPOD and will prove the counterparts of Lemmas 14 and 21. The alternative of one-step contraction in (87a) is easy to obtain by the nature of Proxskip. However, establishing the alternative of (87b) requires the bound for \( \mathbb{E}[\|x^{k+1} - x^k\|^2] \). Unlike the update rule for AiPOD (60) and E-AiPOD (78), the UL update of E2-AiPOD can not be expressed as

\[ x^{k+1} = x^k - \alpha (I - B^1 B) d_f^k \]

unless \( k \mod T = 0 \). However, only this type of error \( \|\alpha (I - B^1 B) d_f^k\|^2 = \alpha^2 \|d_f^k\|^2 \) can be mitigated by the descent of UL. We then observe that the update of virtual sequence in (104) is preferable since \( \mathbb{E}[\|\bar{x}^{k+1} - \bar{x}^k\|^2] = \alpha^2 \mathbb{E}[\|d_f^k\|^2] \). Thus, a corresponding modification is made on the one-step contraction part that we change the reference point from \( y^*(x^k) \) to \( y^*(\bar{x}^k) \). Fortunately, the error induced by treating \( y^{k+1} \) as the output of biased Proxskip with respect to \( y^*(\bar{x}^k) \) is negligible in the final convergence (i.e. \( \mathcal{O}(\beta \alpha^2 T^2 S) \) in (111a)). Formally, we have the following lemma.

**Lemma 27 (Error of LL update).** Suppose that Assumption 1–4 hold and \( \beta \leq \frac{1}{\ell g_1} \), if we choose

\[ N = \mathcal{O}(1/\alpha), \rho \leq \min \left\{ \frac{1}{\ell g_1}, \frac{\mu g}{4 \sigma_{g,2}} \right\} \]

and \( q = \sqrt{\rho \mu_g/2} \), the error of LL update can be bounded by

\[ \mathbb{E}[\|y^{k+1} - y^*(\bar{x}^k)\|^2 + \frac{\beta^2}{p^2} \|r^{k+1} - r^*(\bar{x}^k)\|^2] \]

\[ \leq (1 - \nu)S \mathbb{E}[\|y^* - y^*(\bar{x}^k)\|^2 + \frac{\beta^2}{p^2} \|r^* - r^*(\bar{x}^k)\|^2] + S \beta^2 \sigma_{g,2}^2 + \mathcal{O}(\beta \alpha^2 T^2 S) \]  

\[ \mathbb{E}[\|y^{k+1} - y^*(\bar{x}^k)\|^2] \leq (1 + \gamma + L_{yx} (C_{f,2}^2 + \sigma_{f,2}^2) \alpha^2) \mathbb{E}[\|y^{k+1} - y^*(\bar{x}^k)\|^2] \]

\[ + \left( L_y^2 + L_{yx} \right) \alpha^2 \sigma_{f,2}^2 + \left( L_y^2 + L_{yx} + \frac{L^2}{\gamma} \right) \alpha^2 \mathbb{E}[\|\bar{d}_f^k\|^2] \]

\[ \mathbb{E}[\|r^{k+1} - r^*(\bar{x}^k)\|^2] \leq (1 + \gamma + L_{rx} (C_{f,2}^2 + \sigma_{f,2}^2) \alpha^2) \mathbb{E}[\|r^{k+1} - r^*(\bar{x}^k)\|^2] \]

\[ + \left( L_r^2 + L_{rx} \right) \alpha^2 \sigma_{f,2}^2 + \left( L_r^2 + L_{rx} + \frac{L^2}{\gamma} \right) \alpha^2 \mathbb{E}[\|\bar{d}_f^k\|^2] \]

where \( C_{f,2}^2, \sigma_{f,2}^2 \) are constants defined in Lemma 24, \( \nu := \min \left\{ \beta \mu_g/2, p^2 \right\} \), \( \gamma \) is the balancing parameter that will be chosen in the final theorem.

**Proof:** The proof of (111a) can be viewed as a biased version of (87a) if we treat \( \nabla_y g(x^k, y^k; \phi^{k,s}) \) as a biased estimator of \( \nabla y g(\bar{x}^k, y^k; \phi^{k,s}) \). Note that Lemma C.1 in Proxskip holds even if the gradient estimator is biased since it only considers the randomness of \( \theta^{k,s} \) and uses the properties of projection. Therefore, leveraging Lemma C.1 from Proxskip [50], we get

\[ \mathbb{E}_{\theta^{k,s}} \left[ \|y^{k+1} - y^*(\bar{x}^k)\|^2 + \frac{\beta^2}{p^2} \|r^{k,s+1} - r^*(\bar{x}^k)\|^2 \right] \]
\begin{align*}
\| y^{k,s} - \beta \nabla_y g(x^k, y^{k,s}; \phi^k) - (y^*(\bar{x}^k) - \beta \nabla_y g(\bar{x}^k, y^*(\bar{x}^k))) \|^2 &+ \frac{1 - p^2 \beta^2}{p^2} \| r^{k,s} - r^*(\bar{x}^k) \|^2. \tag{112}
\end{align*}

Then taking a conditional expectation over (112) yields
\begin{align*}
\mathbb{E} \left[ \| y^{k,s} - \beta \nabla_y g(x^k, y^{k,s}; \phi^k) - (y^*(\bar{x}^k) - \beta \nabla_y g(\bar{x}^k, y^*(\bar{x}^k))) \|^2 \left| F_k \right. \right] \\
&\leq (a) \| y^{k,s} - \beta \nabla_y g(x^k, y^{k,s}) - (y^*(\bar{x}^k) - \beta \nabla_y g(\bar{x}^k, y^*(\bar{x}^k))) \|^2 \\
&\quad + \beta^2 \mathbb{E} \left[ \| \nabla_y g(x^k, y^{k,s}, \phi^{k,s}) - \nabla_y g(x^k, y^{k,s}) \|^2 \left| F_k \right. \right] \\
&\leq (b) (1 + \frac{\beta \mu_g}{2}) \| y^{k,s} - \beta \nabla_y g(x^k, y^{k,s}) - (y^*(\bar{x}^k) - \beta \nabla_y g(\bar{x}^k, y^*(\bar{x}^k))) \|^2 \\
&\quad + (1 + \frac{1}{2\beta \mu_g}) \beta^2 \| \nabla_y g(x^k, y^{k,s}) - \nabla_y g(x^k, y^{k,s}) \|^2 + \beta^2 \sigma_g^2 \\
&\leq (c) (1 + \mu_g/2)(1 - \mu_g) \| y^{k,s} - y^*(\bar{x}^k) \|^2 + (1 + \frac{1}{2\mu_g}) \beta^2 \ell_{g,1}^2 \| x^k - \bar{x}^k \|^2 + \beta^2 \sigma_g^2 \tag{113}
\end{align*}

where (a) comes from Lemma 5, (b) is obtained by Young’s inequality, and (c) is derived similarly to (65) and the Lipschitz continuity of \( \nabla_y g(x, y) \).

Furthermore, taking expectation over (113) yields
\begin{align*}
\mathbb{E} \left[ \| y^{k,s} - \beta \nabla_y g(x^k, y^{k,s}; \phi^k) - (y^*(\bar{x}^k) - \beta \nabla_y g(\bar{x}^k, y^*(\bar{x}^k))) \|^2 \right] \\
&\leq (1 + \mu_g/2)(1 - \mu_g) \mathbb{E} \| y^{k,s} - y^*(\bar{x}^k) \|^2 + (1 + \frac{1}{2\mu_g}) \beta^2 \ell_{g,1}^2 \mathbb{E} \| x^k - \bar{x}^k \|^2 + \beta^2 \sigma_g^2 \\
&\leq (1 - \mu_g/2) \mathbb{E} \| y^{k,s} - y^*(\bar{x}^k) \|^2 + O(\alpha^2 T^2) + \beta^2 \sigma_g^2 \tag{114}
\end{align*}

where the last inequality is derived from Lemma 25.

Therefore, combining with (112) and telescoping (114), we get
\begin{align*}
\mathbb{E} \left[ \| y^{k+1} - y^*(\bar{x}^k) \|^2 + \frac{\beta^2}{p^2} \| r^{k+1} - r^*(\bar{x}^k) \|^2 \right] \\
&\leq (1 - \nu)^S \mathbb{E} \left[ \| y^k - y^*(\bar{x}^k) \|^2 + \frac{\beta^2}{p^2} \| r^k - r^*(\bar{x}^k) \|^2 \right] + S \beta^2 \sigma_{g,1}^2 + O(\beta^2 \alpha^2 T^2 S) \tag{115}
\end{align*}

where \( \nu := \min\{\beta \mu_g/2, p^2\} \).

The proof of (111b) is identical to the proof of (63b) by replacing \( \bar{h}_f, \bar{\sigma}_f^2, \bar{C}_f^2 \) by \( \bar{\sigma}_f, \bar{\sigma}_{f,2}^2, (C_{f,1} + \bar{\sigma}_{f,2}^2) \) owing to the update rule in (104). While the proof of (111c) can be obtained with the same spirits of (87b) by replacing \( L_y, L_{yx} \) in (111b) with \( L_r \) and \( L_{rx} \).

\section*{D.5 Proof of Theorem 3}
First, without loss of generality, we can assume that \( \ell_{g,1} \geq 1 \) so that \( L_r \geq L_y, L_{rx} \geq L_{yx} \) and plugging (111b), (111c) into (111a) in Lemma 27, we get that
\begin{align*}
\mathbb{E} \left[ \| y^{k+1} - y^*(\bar{x}^{k+1}) + \frac{\beta^2}{p^2} \| r^{k+1} - r^*(\bar{x}^{k+1}) \|^2 \right]
\end{align*}
Then using Lyapunov function defined in (19) and applying (116), and Lemma 26, we get

\[ E \left[ \mathbb{V}_2^{k+1} \right] - E \left[ \mathbb{V}_2^k \right] \]

\[ \leq \frac{\alpha}{2} E \left[ \left\| \nabla F(\tilde{x}^k) \right\|_{\mathbb{P}_k}^2 \right] + \frac{3\alpha L^2}{2} E \left[ \left\| y^{k+1} - y^*(\tilde{x}^k) \right\|_2^2 \right] + O(\alpha^3 T^2) \]

\[ - \left( \frac{\alpha}{2} - \frac{L_F\alpha^2}{2} \right) E \left[ \left\| d_T^k \right\|_{\mathbb{P}_k}^2 \right] + \frac{L_F\alpha^2\sigma_{g,1}^2}{2} \left( 1 - \rho\mu_g/2 \right) N^2 C^2_u + \frac{2\rho\sigma^2_g}{\mu_g} \]

\[ + \frac{L_f}{L_r} \left( 1 + \frac{\beta^2}{\mu_g} \right) \theta_{\alpha}^2 \sigma_{g,1}^2 + O(\alpha^3 T^2) \]

\[ + \frac{L_f}{L_r} \left( 1 + \frac{\gamma}{\mu_g} \right) \left( 1 + \frac{\beta^2}{\mu_g} \right) \theta_{\alpha}^2 \sigma_{g,1}^2 + O(\alpha^3 T^2) \]

\[ + \frac{L_f L_r}{L_r} \left( 1 + \frac{\gamma}{\mu_g} \right) \left( 1 + \frac{\beta^2}{\mu_g} \right) \theta_{\alpha}^2 \sigma_{g,1}^2 + O(\alpha^3 T^2) \]

\[ \leq \frac{\alpha}{2} E \left[ \left\| \nabla F(\tilde{x}^k) \right\|_{\mathbb{P}_k}^2 \right] + \frac{L_f}{L_r} \left( 1 + \frac{11L_f L_r \alpha}{2} \right) \theta_{\alpha}^2 \sigma_{g,1}^2 + O(\alpha^3 T^2) \]

\[ + \frac{L_f L_r}{L_r} \left( 1 + \frac{2\beta}{\mu_g} \right) \theta_{\alpha}^2 \sigma_{g,1}^2 + O(\alpha^3 T^2) \]

\[ - \frac{\alpha}{4} - \left( \frac{L_f}{2} + L_f L_r + \frac{L_f L_r}{L_r} \right) \theta_{\alpha}^2 - \frac{\beta \alpha}{2\mu_g} - \left( L_f L_r + \frac{L_f L_r}{L_r} \right) \frac{2\beta\alpha^2}{\mu_g} \]

\[ \mathbb{E} \left[ \left\| d_T^k \right\|_{\mathbb{P}_k}^2 \right] \]

Selecting \( \gamma = 4L_f L_r \alpha \) and \( p = \sqrt{\beta\mu_g/2} \), (117) can be simplified by

\[ \mathbb{E}[\mathbb{V}_2^{k+1}] - \mathbb{E}[\mathbb{V}_2^k] \leq -\frac{\alpha}{2} E \left[ \left\| \nabla F(\tilde{x}^k) \right\|_{\mathbb{P}_k}^2 \right] + \frac{L_f}{L_r} \left( 1 + \frac{11L_f L_r \alpha}{2} \right) \theta_{\alpha}^2 \sigma_{g,1}^2 + O(\alpha^3 T^2) \]

\[ + \frac{L_f L_r}{L_r} \left( 1 + \frac{2\beta}{\mu_g} \right) \theta_{\alpha}^2 \sigma_{g,1}^2 + O(\alpha^3 T^2) \]

\[ - \frac{\alpha}{4} - \left( \frac{L_f}{2} + L_f L_r + \frac{L_f L_r}{L_r} \right) \theta_{\alpha}^2 - \frac{\beta \alpha}{2\mu_g} - \left( L_f L_r + \frac{L_f L_r}{L_r} \right) \frac{2\beta\alpha^2}{\mu_g} \]

As before, we can choose \( \beta = O(\alpha) \) to make the last two terms non-positive. Specifically, a sufficient condition for this is to choose \( \beta = c_1 \alpha \) and \( \alpha \leq \min(\alpha_1, \alpha_2) \) where

\[ c_1 = \frac{11L_f L_r + 2L_f L_r (C_{f,2}^2 + \sigma_{f,2}^2)}{\mu_g} \]

\[ \alpha_1 = \frac{1}{c_1 \ell_{g,1}} \]
Additionally, we set \( N = O(1/\alpha) \) such that \((1 - \rho \mu_g / 2)^N = O(\alpha^2)\), then (118) becomes
\[
\frac{\alpha}{2} \mathbb{E}[\|\nabla F(x^k)\|_{p_x}^2] \leq \left( \mathbb{E}[\|\nabla F^0\|_{p_x}^2] \right) + O(\alpha^2\sigma^2_{g,1} + S\alpha^2 T^2 + \alpha^2 \sigma^2_{f,2} + \rho \alpha \sigma^2_u).
\](119)

Telescoping (119) and dividing both sides by \( \alpha K / 2 \) yields
\[
\frac{1}{K} \sum_{k=0}^{K-1} \mathbb{E}[\|\nabla F(x^k)\|_{p_x}^2] \leq \frac{2(\mathbb{E}[\|\nabla F^0\|_{p_x}^2] - \mathbb{E}[\|\nabla F^k\|_{p_x}^2])}{\alpha K} + O(S\alpha^2\sigma^2_{g,1} + S\alpha^2 T^2 + \alpha^2 \sigma^2_{f,2} + \rho \alpha \sigma^2_u).
\]

Choosing \( \alpha = O\left(\frac{1}{\sqrt{K}}\right) \), \( S = O(1) \), \( T = O(K^{1/4}) \) and \( \rho = O\left(\frac{1}{\sqrt{K}}\right) \) leads to Corollary 3.

E Application on Federated Bilevel Learning

In this section, we present the pseudo-code of E-AiPOD and E2-AiPOD for federated bilevel learning and compare the metric we used with the state-of-the-art works.

E.1 Pseudo-code of E-AiPOD and E2-AiPOD on federated bilevel learning

The application of E2-AiPOD in the federated bilevel setting is straightforward with the facts in Section 5. For E-AiPOD, if we plug \( V_2 \) in (22) to (9a), then we obtain \( w^k = [w^k_1, \ldots, w^k_M] \) with
\[
\frac{1}{M} \sum_{m=1}^{M} \nabla_g f(x^k_m, y^{k+1}_m; \phi_{(0)}) \left( \frac{cN}{\ell_{g,1}} \prod_{n=1}^{N'} \left( I - \frac{\tilde{c}}{M\ell_{g,1}} \sum_{m=1}^{M} \nabla_{y g} g(x^k_m, y^{k+1}_m; \phi_{(n)}) \right) \right) \times \left( \frac{1}{M} \sum_{m=1}^{M} \nabla_{y f}(x^k_m, y^{k+1}_m; \phi_{(m)}) \right).
\](120)

To avoid transmission of Hessian, which is highly expensive, we can calculate \( w^k_m \) by communicating the Hessian-vector product purely like in FedNest [57], which is detailed in Algorithm 8. We summarize E-AiPOD and E2-AiPOD on federated bilevel learning together in Algorithm 6.

E.2 Equivalence between our metric with metric in federated bilevel learning

In this section, we prove the equivalence of our measure in (4) with the measure of FedNest in non-consensus federated bilevel setting.

According to Lemma 6, and \( \mathcal{X} = \{x \mid Bx = 0\} \) in federated bilevel setting, we know
\[
(I - B^\dagger B)\nabla F(x) = \text{Proj}_{\mathcal{X}}(\nabla F(x)).
\](121)

Then according to (24a) and (23a), we obtain
\[
(I - B^\dagger B)\nabla F(x) = \frac{1}{M} \sum_{m=1}^{M} \nabla_{x m} f_m(x_m, y^*_m(x_m)) + \frac{1}{M} \sum_{m=1}^{M} \nabla_{x m} g_m(x_m, y^*_m(x_m))
\]

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\begin{algorithm}
\caption{E-AiPOD and E2-AiPOD in federated bilevel learning: blue part is run only by E-AiPOD; red part is implemented only by E2-AiPOD; not both at the same time.}
\begin{algorithmic}
\State Initialization: \( \{x^0_m, y^0_m\}_{m \in [M]} \), stepsizes \( \{\alpha, \beta, \delta, \rho\} \), projection probability \( \{p, q\} \), projection frequency \( T \)
\For {\( k = 0 \) to \( K - 1 \)}
\State \( \{y^{k+1}_m, r^{k+1}_m\}_{m \in [M]} = \text{E-AiPOD}^{\text{low}}(\{x^k_m, y^k_m, r^k_m\}_{m \in [M]}; \beta, p, S) \)
\State call Algorithm 8 to calculate \( \{w^k_m\}_{m \in [M]} \)
\For {all workers \( m \in [M] \) in parallel}
\State \( x^{k+1}_m = x^k_m \)
\State \( \text{for } t = 0 \) to \( T - 1 \) do
\State \( x^{k,t+1}_m = x^{k,t}_m - \alpha(\nabla_x f_m(x^{k,t}_m; y^k_m, z^k_m) - w^k_m) \)
\EndFor
\State \( \Delta^k_m = x^{k,T}_m - x^k_m \)
\State \( x^{k+1} = x^k + \delta \sum_{m=1}^{M} \Delta^k_m \)
\EndFor
\EndFor
\State \( \{u^{k+1}_m\}_{m \in [M]} = \text{E-AiPOD}^{\text{med}}(\{x^k_m, y^{k+1}_m\}_{m \in [M]}; \rho, q, N) \)
\For {all workers \( m \in [M] \) in parallel}
\State \( x^{k+1}_m = x^k_m - \alpha(\nabla_x f_m(x^{k+1}_m; y^k_m, z^k_m) + \nabla_{xy} g_m(x^{k+1}_m; y^k_m; \phi^k_m)u^{k+1}_m) \)
\EndFor
\If {\( K \mod T = 0 \)}
\State \( x^{k+1} = \frac{1}{M} \sum_{i=1}^{M} x^{k+1}_i \)
\EndIf
\EndFor
\end{algorithmic}
\end{algorithm}

\begin{algorithm}
\caption{E-AiPOD^{\text{med}}(\{x^k_m, y^k_m, r^k_m\}_{m \in [M]}, \beta, p, S): green part denotes the communication round}
\begin{algorithmic}
\State Initialization: \( \{x^k_m, y^k_m, r^k_m\}_{m \in [M]} \), stepsize \( \beta \), skipping probability \( p \), \( y^{k,0}_m = y^k_m, r^{k,0}_m = r^k_m, \forall m \in [M] \)
\For {\( s = 0 \) to \( S - 1 \)}
\State \textbf{for} all workers \( m \in [M] \) \textbf{in parallel} do
\State \( \hat{g}^{k,s+1}_m = g^{k,s}_m - \beta(\nabla_y g_m(x^{k,s}_m, y^{k,s}_m; \phi^{k,s}_m) - r^{k,s}_m) \)
\State \If {a Bernoulli random variable \( \theta^{k,s} = 1 \)} \Comment{\( \mathbb{P}(\theta^{k,s} = 1) = p \)}
\State \( \hat{y}^{k+1}_m = \frac{1}{M} \sum_{i=1}^{M} \left( \hat{g}^{k+1}_i - \frac{\theta^{k,s}_i}{p_i} \right) \) \Comment{Communicate to server and average}
\State \( r^{k,s+1}_m = g^{k,s}_m + \frac{\beta}{p_i} (\hat{y}^{k+1}_m - y^{k,s+1}_m) \)
\Else \Comment{\( \theta^{k,s} = 0 \)}
\State \( y^{k,s+1}_m = \hat{y}^{k+1}_m, \quad r^{k,s+1}_m = r^{k,s}_m \)
\EndIf
\EndFor
\State Outputs: \( \{y^{k+1}_m, r^{k+1}_m\}_{m \in [M]} \)
\EndFor
\end{algorithmic}
\end{algorithm}

\begin{equation}
\left( \frac{1}{M} \sum_{m=1}^{M} \nabla_{y_m} y_m g_m(x_m, y^*_m(x_m)) \right)^{-1} \left( \frac{1}{M} \sum_{m=1}^{M} \nabla_{y_m} f_m(x_m, y^*_m(x_m)) \right).
\end{equation}

On the other hand, the gradient of the objective in FedNest is

\begin{equation}
\frac{1}{M} \sum_{m=1}^{M} \nabla_x f_m(x, y^*(x)) + \left( \frac{1}{M} \sum_{m=1}^{M} \nabla_{xy} g_m(x, y^*(x)) \right).
\end{equation}
We find that (123) is the same as (122), if replacing $g_m(x, y^*(x))$ and $f_m(x, y^*(x))$ by $g_m(x_m, y_m^*(x_m))$ and $f_m(x_m, y_m^*(x_m))$. Moreover, since $\mathbb{E}[\|\nabla F(x)\|_F^2] = \mathbb{E}[(I - B^T B)\|\nabla F(x)\|^2]$, the measure $\mathbb{E}[\|\nabla F(x)\|_F^2]$ in our analysis coincides with the gradient norm measure in FedNest [57].

F Additional Details of Experiments

We will report the detailed settings of the experiments in Section 6. In the federated bilevel learning experiments, the number of workers is set as $M = 50$ and each local network is a 2-layer multilayer perceptron with hidden dimension 200. The hyper-parameters are found by measuring both the convergence speed and the stability of the algorithm via a grid search.
Synthetic task. E-AiPOD: The projection probability is set as $p = 0.3$ in the right figures, the total number of iterations is $K = 400/p$, the number of UL iterations is $T = 2$ in the left figures, the number of LL iterations is $S = 5$, the step sizes are set as $\alpha = 0.02, \beta = 0.01$, the noise has mean 0 and std 0.1. AiPOD is a special case of E-AiPOD with $p = 1$.

Federated hyper-representation learning. E-AiPOD: The communication probability is set as $p = 0.1$ in Figure 2 (right), $S = 20, \alpha = 0.01, \beta = 0.05$, Neumann iteration $N' = 5$, and the batch size is 256. FedNest (notations in [57]): Choose LL iteration number $\tau = 10$ and episode $T = 1$ so that the communication frequency is 0.1 per LL iteration, which is the same as the choice of $p$ for E-AiPOD. The UL iteration numbers are specified in Figure 2, and we set $\alpha = 0.01, \beta = 0.02$ (under $T = 1$) or $\beta = 0.01$ (under $T = 5$), $N' = 5$ and batch size as 256.

Federated learning from imbalanced data-set. E-AiPOD: Communication probability $p = 0.3$ in Figure 2 (right), $S = 20, \alpha = 0.01, \beta = 0.04, N' = 3$, and batch size 256. FedNest: Choose LL iteration number $\tau = 3$ and episode $T = 3$ and thus the communication frequency is 0.3 per LL iteration, which is the same as $p = 0.3$. The UL iteration numbers are specified in Figure 2. Set $\alpha = 0.01, \beta = 0.02, N' = 3$, and batch size as 256.