An Accelerated Algorithm for Stochastic Bilevel Optimization under Unbounded Smoothness

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Abstract

This paper investigates a class of stochastic bilevel optimization problems where the upper-level function is nonconvex with potentially unbounded smoothness and the lower-level problem is strongly convex. These problems have significant applications in sequential data learning, such as text classification using recurrent neural networks. The unbounded smoothness is characterized by the smoothness constant of the upper-level function scaling linearly with the gradient norm, lacking a uniform upper bound. Existing state-of-the-art algorithms require $\widetilde{O}(\epsilon^{-4})$ oracle calls of stochastic gradient or Hessian/Jacobian-vector product to find an ϵ-stationary point. However, it remains unclear if we can further improve the convergence rate when the assumptions for the function in the population level also hold for each random realization almost surely (e.g., Lipschitzness of each realization of the stochastic gradient). To address this issue, we propose a new Accelerated Bilevel Optimization algorithm named AccBO. The algorithm updates the upper-level variable by normalized stochastic gradient descent with recursive momentum and the lower-level variable by the stochastic Nesterov accelerated gradient descent algorithm with averaging. We prove that our algorithm achieves an oracle complexity of $\widetilde{O}(\epsilon^{-3})$ to find an ϵ-stationary point, when the lower-level stochastic gradient has a small variance $O(\epsilon)$. Our proof relies on a novel lemma characterizing the dynamics of stochastic Nesterov accelerated gradient descent algorithm under distribution drift with high probability for the lower-level variable, which is of independent interest and also plays a crucial role in analyzing the hypergradient estimation error over time. Experimental results on various tasks confirm that our proposed algorithm achieves the predicted theoretical acceleration and significantly outperforms baselines in bilevel optimization. The code is available here.

1 Introduction

Bilevel optimization receives tremendous attention recently in the machine learning community, due to its applications in meta-learning [27, 59], hyperparameter optimization [27, 25], data hyper-cleaning [44], continual learning [7, 37], and reinforcement learning [47]. The bilevel optimization problem has the following formulation:

$$\min_{x\in\mathbb{R}^{d_x}} \Phi(x) := f(x, y^*(x)), \text{ s.t., } y^*(x) \in \arg\min_{y\in\mathbb{R}^{d_y}} g(x, y), \tag{1}$$

where f and g are upper-level and lower-level functions respectively. For example, in meta-learning [26, 27], x denotes the layers of neural networks for shared representation learning, y denotes the task-specific head encoded in the last layer, and the formulation (1) aims to learn the a common representation learning encoder x such that it can be quickly adapted to downstream tasks

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by only updating the task-specific head y. In machine learning, people typically consider stochastic optimization setting such that $f(x,y) = \mathbb{E}_{\xi\sim\mathcal{D}_f}[F(x,y;\xi)]$ and $g(x,y) = \mathbb{E}_{\zeta\sim\mathcal{D}_g}[G(x,y;\zeta)]$, where $\mathcal{D}_f$ and $\mathcal{D}_g$ are the underlying unknown data distributions for f and g respectively, and one can access noisy observations of f and g based on sampling from $\mathcal{D}_f$ and $\mathcal{D}_g$.

There emerges a wave of studies for algorithmic design and analysis for solving the bilevel optimization problem (1) under different assumptions of f and g. Most theoretical work assumes the upper-level function is smooth (i.e., gradient is Lipschitz) and nonconvex, and the lower-level function is strongly convex [30, 44, 41, 33, 48]. However, as pointed out by [75, 15], certain neural networks such as recurrent neural networks [22], long-short term memory networks [40] and transformers [65] have smoothness constants that scale with gradient norm, potentially leading to unbounded smoothness constants (i.e., gradient Lipschitz constant can be infinity). Motivated by this, Hao et al. [38] designed the first bilevel optimization algorithm to handle the cases where f is nonconvex with potentially unbounded smoothness and g is strongly convex. The algorithm in [38] achieves $\widetilde{O}(\epsilon^{-4})$ oracle complexity for finding an ϵ-stationary point (i.e., a point x such that $\|\nabla\Phi(x)\| \leq \epsilon$). Gong et al. [32] proposed an single-loop algorithm under the same setting as in [38] and also achieved $\widetilde{O}(\epsilon^{-4})$ oracle complexity. This complexity result is worse than the $\widetilde{O}(\epsilon^{-3})$ oracle complexity under the relatively easier setting where f has a Lipschitz gradient, and each realization of the stochastic oracle calls is Lipschitz with respect to its argument (e.g., almost-sure Lipschitz oracle) [71, 46, 18, 34, 43]. This naturally motivates us to study the following question:

Is it possible to improve the $\widetilde{O}(\epsilon^{-4})$ oracle complexity for bilevel optimization problems where the upper-level function is nonconvex with unbounded smoothness and the lower-level function is strongly convex, by assuming that the properties of the function at the population level also hold almost surely for each random realization?

In this paper, we give a positive answer to this question by designing a new algorithm named AccBO with an improved oracle complexity of $\widetilde{O}(\epsilon^{-3})$, when the lower-level stochastic gradient has a small variance $O(\epsilon)$. Our algorithm is inspired by momentum-based variance reduction techniques used in nonconvex smooth optimization [18] under the almost-sure Lipschitz stochastic gradient oracle framework. The innovation of AccBO lies in its update rules: it employs normalized stochastic gradient descent with recursive momentum for the upper-level variable and stochastic Nesterov accelerated gradient descent with averaging for the lower-level variable. Our approach differs from existing accelerated bilevel optimization algorithms, such as those proposed by [71, 46] in two key ways: (i) while these algorithms use recursive momentum for the upper-level variable update, AccBO utilizes normalized recursive momentum to address the unbounded smoothness of the upper-level function; (ii) for the lower-level variable update, we use stochastic Nesterov accelerated gradient descent with averaging, in contrast to the recursive momentum method used by the other algorithms. The primary challenge in analyzing the convergence rate of AccBO arises from the need to simultaneously control errors from both upper-level and lower-level variables, given the unbounded smoothness, large learning rate, and recursive momentum in the upper-level problem. Our main contributions are summarized as follows.

- We design a new algorithm named AccBO for solving bilevel optimization problems where the upper-level function is nonconvex with unbounded smoothness and the lower-level function is strongly convex. AccBO leverages normalized recursive momentum for the upper-level variable and Nesterov momentum for the lower-level variable under the stochastic setting to achieve acceleration. To the best of our knowledge, the simultaneous usage of these two techniques in stochastic bilevel optimization is novel and has not been previously explored in the bilevel optimization literature.
- We prove that the AccBO algorithm requires $\widetilde{O}(\epsilon^{-3})$ oracle calls for finding an ϵ-stationary point, when the variance of the lower-level stochastic gradient is $O(\epsilon)$. This complexity strictly improves the state-of-the-art oracle complexity for unbounded smooth nonconvex upper-level problem and strongly-convex lower-level problem as described in [38, 32] [2]. To achieve this result, we introduce novel proof techniques for analyzing the dynamics of stochastic Nesterov accelerated gradient descent under distribution drift with high probability

[2]Note that even if the lower-level stochastic gradient variance is $O(\epsilon)$, the oracle complexity required in [38, 32] is still $\widetilde{O}(\epsilon^{-4})$ since the oracle complexity required for their upper-level problem is already $\widetilde{O}(\epsilon^{-4})$.

for the lower-level variable, which are crucial for analyzing the hypergradient error and also of independent interest.

- We empirically verify the effectiveness of our proposed algorithm on various tasks, including deep AUC maximization and data hypercleaning. Our algorithm indeed achieves the predicted theoretical acceleration and significantly outperforms baselines in bilevel optimization.

2 Related Work

Relaxed Smoothness. The concept of relaxed smoothness was initially introduced by [75], inspired by the loss landscapes observed in recurrent neural networks and long-short term memory networks. They show that techniques such as gradient clipping and normalization could improve the performance compared with gradient descent in these scenarios. It inspired further investigations that concentrate on various aspects, including improved analysis on gradient clipping and normalization [74, 45], adaptive algorithms [15, 51, 68, 24], federated algorithms [54, 16, 17], generalized assumptions [15, 14], and recursive momentum based methods with faster rates [60, 56]. The work of [38, 32] considered a relaxed smoothness condition for the upper-level problem in the bilevel optimization setting.

Bilevel Optimization. Bilevel optimization refers to a special kind of optimization where one problem is embedded within another. It was first introduced by [9]. Early works developed specific bilevel optimization algorithms with asymptotic convergence analysis [67, 1, 69]. Ghadimi and Wang [30] initiated the study of non-asymptotic convergence for gradient-based methods in bilevel optimization where the upper-level problem is smooth and the lower-level problem is strongly convex. This field saw further advancements with improved complexity results [41, 44, 11, 21, 12] and fully first-order algorithms [48, 52]. There is a line of work which leverages almost-sure Lipschitz oracle (e.g., stochastic gradient) to obtain improved convergence rates of bilevel optimization algorithms [71, 46]. When the lower-level function is not strongly convex, several algorithmic framework and approximation schemes were proposed [61, 63, 49, 62, 55, 10]. The setting considered in this paper is very close to [38, 32], where the upper-level function is nonconvex and unbounded smooth, and the lower-level function is strongly convex. However, the work of [38, 32] do not have an accelerated rate $\widetilde{O}(\epsilon^{-3})$ for finding an ϵ-stationary point as established in this paper.

Nesterov Accelerated Gradient and Variants. Nesterov Accelerated Gradient (NAG) method was introduced by [58] for deterministic convex optimization problems. The stochastic version of NAG (SNAG) was extensively studied in the literature [3, 5, 66, 13]. To the best of our knowledge, none of them provide a high probability analysis for SNAG. In the online learning setting, there is a line of work focusing on the perspective of sequential stochastic/online optimization with distributional drift [6, 70, 57, 20]. While these studies provide valuable insights into adaptive techniques and performance bounds under distributional drift, they do not explore the potential integration of such methods with bilevel optimization problems, nor do they consider the application of SNAG within this framework.

3 Problem Setup and Preliminaries

Define $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ as the inner product and the Euclidean norm. Throughout the paper, we use asymptotic notation $\widetilde{O}(\cdot)$, $\widetilde{\Theta}(\cdot)$, $\widetilde{\Omega}(\cdot)$ to hide polylog factors in ϵ^{-1} and $1/\delta$. Denote $f\colon \mathbb{R}^{d_x} \times \mathbb{R}^{d_y} \to \mathbb{R}$ as the upper-level function, and $g\colon \mathbb{R}^{d_x} \times \mathbb{R}^{d_y} \to \mathbb{R}$ as the lower-level function. The hypergradient $\nabla \Phi(x)$ has the following form [30]:

$$\nabla \Phi(x) = \nabla_x f(x, y^*(x)) - \nabla^2_{xy} g(x, y^*(x)) \left[\nabla^2_{yy} g(x, y^*(x))\right]^{-1} \nabla_y f(x, y^*(x)). \tag{2}$$

To avoid the Hessian inverse computation, we typically use the following Neumann series to approximate the hypergradient [30, 46, 41]. In particular, for the stochastic setting, define

$$\bar{\nabla} f(x, y; \bar{\xi}) = \nabla_x F(x, y; \xi) - \frac{Q}{l_{g,1}} \nabla^2_{xy} G(x, y; \zeta^{(0)}) \prod_{i=1}^{\mathsf{q}(Q)} \left(I - \frac{\nabla^2_{yy} G(x, y; \zeta^{(i)})}{l_{g,1}} \right) \nabla_y F(x, y; \xi),$$

where $\mathsf{q}(Q) \sim \mathrm{Uniform}\{0, \ldots, Q-1\}$, $\bar{\xi} := \{\xi, \zeta^{(0)}, \ldots, \zeta^{(\mathsf{q}(Q))}\}$ and we use the convention that $\prod_{i=1}^{j} A_i = I$ if $j = 0$. Then $\mathbb{E}_{\bar{\xi}}[\bar{\nabla} f(x, y; \bar{\xi})]$ is a good approximation of $\nabla \Phi(x)$ if y and $y^*(x)$ are close [30].

Throughout the paper, we make the following assumptions.

Assumption 3.1 (($L_{x,0}, L_{x,1}, L_{y,0}, L_{y,1}$)-smoothness [38]). *Let $z = (x, y)$ and $z' = (x', y')$, there exists $L_{x,0}, L_{x,1}, L_{y,0}, L_{y,1} > 0$ such that for all z, z', if $\|z - z'\| \leq 1/\sqrt{2(L_{x,1}^2 + L_{y,1}^2)}$, then $\|\nabla_x f(z) - \nabla_x f(z')\| \leq (L_{x,0} + L_{x,1}\|\nabla_x f(z)\|)\|z - z'\|$ and $\|\nabla_y f(z) - \nabla_y f(z')\| \leq (L_{y,0} + L_{y,1}\|\nabla_y f(z)\|)\|z - z'\|$.*

Remark: Assumption 3.1 is introduced by [38] for describing the bilevel optimization problems with recurrent neural networks. This assumption can be regarded as a block-wise relaxed smoothness assumptions for two blocks x and y, which is a variant of the relaxed smoothness assumption [75] and the coordinate-wise relaxed smooth assumption [15].

Assumption 3.2. *Suppose the followings hold for objective functions f and g: (i) f is continuously differentiable and $(L_{x,0}, L_{x,1}, L_{y,0}, L_{y,1})$-smooth in (x, y); (ii) For every x, $\|\nabla_y f(x, y)\| \leq l_{f,0}$ for all y; (iii) For every x, $g(x, y)$ is μ-strongly-convex in y for $\mu > 0$; (iv) g is $l_{g,1}$-smooth jointly in (x, y); (v) g is twice continuously differentiable, and $\nabla_{xy}^2 g, \nabla_{yy}^2 g$ are $l_{g,2}$-Lipschitz jointly in (x, y).*

Remark: Assumption 3.2 is standard in the bilevel optimization literature [48, 38, 30]. Assumption 3.2 (i) characterizes the unbounded smoothness of the upper-level function and is empirically observed in recurrent neural networks [38].

Assumption 3.3. *The following stochastic estimators are unbiased and have the following properties:*

$$\mathbb{E}_{\xi\sim\mathcal{D}_f}[\|\nabla_x F(x, y; \xi) - \nabla_x f(x, y)\|^2] \leq \sigma_{f,1}^2, \quad \mathbb{E}_{\xi\sim\mathcal{D}_f}[\|\nabla_y F(x, y; \xi) - \nabla_y f(x, y)\|^2] \leq \sigma_{f,1}^2,$$

$$\Pr(\|\nabla_y G(x, y; \xi) - \nabla_y g(x, y)\| \geq \lambda) \leq 2\exp(-2\lambda^2/\sigma_{g,1}^2) \quad \forall \lambda > 0,$$

$$\mathbb{E}_{\zeta\sim\mathcal{D}_g}[\|\nabla_{xy}^2 G(x, y; \zeta) - \nabla_{xy}^2 g(x, y)\|^2] \leq \sigma_{g,2}^2, \quad \mathbb{E}_{\zeta\sim\mathcal{D}_g}[\|\nabla_{yy}^2 G(x, y; \zeta) - \nabla_{yy}^2 g(x, y)\|^2] \leq \sigma_{g,2}^2.$$

Remark: Assumption 3.3 assumes the stochastic oracle for the upper-level problem has bounded variance, which is standard in nonconvex stochastic optimization [28–30]. It also assumes the stochastic oracle for the lower-level problem is light-tailed, which is common for the high probability analysis for the lower-level problem [50, 39]. Note that the same assumption is also made in [38, 32] for the bilevel problems with a unbounded smooth upper-level function.

Assumption 3.4. *$F(x, y; \xi)$ and $G(x, y; \zeta)$ satisfy Assumption 3.2 for every ξ and ζ almost surely.*

Remark: Assumption 3.4 assumes that each random realization of the upper- and lower-level functions satisfies the same property as in the population level. Note that this condition is the key to achieve an improved $\widetilde{O}(\epsilon^{-3})$ oracle complexity under various settings, including both single-level nonconvex smooth problems [23, 18, 64] and bilevel problems with nonconvex smooth upper-level objectives [71, 46]. Furthermore, this assumption is shown to be necessary for achieving improved oracle complexity in single-level problems [2].

4 Algorithm and Analysis

4.1 Main Challenges and Algorithm Design

Main Challenges. We begin by explaining why existing bilevel optimization algorithms and their corresponding analysis techniques are insufficient in our setting. First, most algorithms developed for bilevel optimization require the upper-level function is smooth (i.e., the gradient of the upper-level function is Lipschitz) [30, 44, 41, 71, 46, 21, 48]. They characterize the estimation error of the optimal solution for the lower-level problem, utilize an approximate hypergradient descent approach and the descent lemma for L-smooth functions to prove the convergence. In particular, they demonstrate that a potential function, incorporating both the function value and the bilevel error from the lower-level problem, progressively decreases in expectation. However, when the upper-level function is $(L_{x,0}, L_{x,1}, L_{y,0}, L_{y,1})$-smooth as illustrated in Assumption 3.1, the previous algorithms and analyses relying on L-smoothness do not work. The reason is that the hypergradient bias depends on the approximation error of the lower-level variable as well as the hypergradient itself: these elements are statistically dependent and the standard potential function argument with an expectation-based analysis would not work. To address this issue, the work of [38, 32] requires a careful high probability analysis in the unbounded smoothness setting and obtains $\widetilde{O}(\epsilon^{-4})$ oracle complexity. Such a requirement of high probability analysis prevents us from leveraging the momentum-based

Algorithm 1 STOCHASTIC NESTEROV ACCELERATED GRADIENT METHOD (SNAG)

Input: $x, \tilde{y}_{-1}, \tilde{y}_0, \tilde{\alpha}, T_0$ # $\texttt{SNAG}(x, \tilde{y}_0, \tilde{\alpha}, T_0)$
for $t = 0, 1, \ldots, T_0 - 1$ **do**
  Sample $\tilde{\pi}_t$ from distribution $\mathcal{D}_g$
  $\tilde{z}_t = \tilde{y}_t + \gamma(\tilde{y}_t - \tilde{y}_{t-1})$
  $\tilde{y}_{t+1} = \tilde{z}_t - \tilde{\alpha}\nabla_y G(x, \tilde{z}_t; \tilde{\pi}_t)$
end for

variance reduction technique for updating the lower-level variable. For example, the work [46] which has $\widetilde{O}(\epsilon^{-3})$ oracle complexity in the smooth case leverages the momentum-based variance reduction technique [18] for updating the lower-level variable with an expectation-based analysis, but it seems difficult to establish a high probability analysis for the momentum-based variance reduction algorithm in terms of the lower-level variable. Second, the recent work of Hao et al. [38] and Gong et al. [32] considered that the upper-level function is unbounded smooth and addressed this issue by performing normalized stochastic gradient with momentum for the upper-level variable and periodic updates or stochastic gradient descent for the lower-level variable, but their oracle complexity is not better than $\widetilde{O}(\epsilon^{-4})$. These facts indicate that we need new algorithm design and analysis techniques to get potential acceleration.

Algorithm Design. To obtain potential acceleration and enable a high probability analysis for the lower-level variable, our key idea is to update the upper-level variable by normalized stochastic gradient descent with recursive momentum and update the lower-level variable by the stochastic Nesterov accelerated gradient (SNAG) method. Different from [38, 32], the key innovation of our algorithm design is that we achieve acceleration for both upper-level and lower-level problems simultaneously but without affecting each other. The upper-level update rule can be regarded as a generalization of the acceleration technique (e.g., the momentum-based variance reduction technique) [18, 56] from single-level to bilevel problems. The main challenge is that we need to deal with the accumulated error of the recursive momentum over time due to the hypergradient bias, which is caused by the inaccurate estimation of the optimal lower-level variable. Therefore we require a very small tracking error between the iterate of the lower-level variable and the optimal lower-level solution defined by the upper-level variable (i.e., $y^*(x)$) at every iteration. This requirement is satisfied by executing SNAG method under the distribution drift for the lower-level problem, where the drift is caused by the change of the upper-level variable over time. Note that we can provide a high probability analysis of the SNAG method under distributional drift, which strictly improves the analysis of SGD under distributional drift in [19] in the small stochastic gradient noise regime.

The detailed description of our algorithm is illustrated in Algorithm 2. At the very beginning, we run a certain number of iterations of SNAG for the fixed upper-level variable x_0 (line 2) as the warm-start stage, and then update the lower-level variable by SNAG (line $8 \sim 20$) with averaging (line 21) and update the upper-level variable by normalized stochastic gradient descent with recursive momentum (line $23 \sim 24$). Note that we have two options for implementing SNAG. In Option I (line $8 \sim 9$), the algorithm simply runs SNAG under distribution drift caused by the sequence $\{x_t\}$. Option I is specifically designed for a particular subset of bilevel optimization problems where the lower-level function is a quadratic function. Option II (line $11 \sim 20$) is designed for a broader range of bilvel optimization problems, accommodating general strongly-convex lower-level functions. In Option II, we run SNAG with periodic updates: the lower-level update is performed for N iterations only when the iteration number t is a multiple of I.

4.2 Main Results

We first introduce some useful notations. Let $\sigma(\cdot)$ be the σ-algebra generated by the random variables in the argument. We define the following filtrations for $t \geq 1$: $\mathcal{F}^{\text{init}} = \sigma(\tilde{\pi}_0, \ldots, \tilde{\pi}_{T_0-1})$, $\mathcal{F}_t = \sigma(\bar{\xi}_0, \ldots, \bar{\xi}_{t-1})$, $\widetilde{\mathcal{F}}_t^1 = \sigma(\pi_0, \ldots, \pi_{t-1})$, and we also define $\widetilde{\mathcal{F}}_t^2 = \sigma(\pi_t^0, \ldots, \pi_t^{N-1})$ when t is a multiple of I. We use $\mathbb{E}_t$, $\mathbb{E}_{\mathcal{F}_t}$ and $\mathbb{E}$ to denote the conditional expectation $\mathbb{E}[\cdot \mid \mathcal{F}_t]$, the expectation over $\mathcal{F}_t$ and the total expectation over $\mathcal{F}_T$ respectively.

Theorem 4.1. *Suppose Assumptions 3.1 to 3.4 hold. Let $\{x_t\}$ be the iterates produced by Algorithm 2. For any given $\delta \in (0, 1)$ and small enough ϵ (see exact choice in* (54)*), if $\sigma_{g,1} = O(\sqrt{\epsilon})$ as defined in* (55)*, and we set parameters $\alpha^{\text{init}}, \alpha, \beta, \gamma, \eta, \tau, I, N, S, Q, T_0$ (see exact choices in* (56)*,* (57)*,* (58)*,*

Algorithm 2 ACCELERATED BILEVEL OPTIMIZATION ALGORITHM (ACCBO)

1: **Input:** $\alpha^{\text{init}}, \alpha, \beta, \gamma, \eta, \tau, I, S, T_0, T$, set $x_0, y_0^{\text{init}} = 0$
2: $y_0 = \texttt{SNAG}(x_0, y_0^{\text{init}}, \alpha^{\text{init}}, T_0)$, and set $y_{-1} = \hat{y}_0 = y_0$ # Warm-start
3: **for** $t = 0, 1, \ldots, T-1$ **do**
4: Sample $\mathsf{q}(Q) \sim \text{Uniform}\{0, \ldots, Q-1\}$ and $\{\zeta_{t,s}^{(0)}, \ldots, \zeta_{t,s}^{(\mathsf{q}(Q))}\}_{s=1}^{S} \sim \mathcal{D}_g$
5: Sample $\{\xi_{t,s}\}_{s=1}^{S} \sim \mathcal{D}_f$, denote $\bar{\xi}_t := \cup_{s=1}^{S}\{\mathsf{q}(Q), \xi_{t,s}, \zeta_{t,s}^{(0)}, \ldots, \zeta_{t,s}^{(\mathsf{q}(Q))}\}$
6: # Lower-Level: Stochastic Nesterov Accelerated Gradient Descent with Averaging
7: # Option I: from Line 8 $\sim$ 9 (for quadratic lower-level function)
8: $z_t = y_t + \gamma(y_t - y_{t-1})$
9: $y_{t+1} = z_t - \alpha \nabla_y G(x_t, z_t; \pi_t)$, where $\pi_t \sim \mathcal{D}_g$
10: # Option II: from Line 11 $\sim$ 20 (for general strongly convex lower-level function)
11: **if** $t > 0$ and t is a multiple of I **then**
12: Set $y_t^0 = y_t^{-1} = y_t$
13: **for** $j = 0, 1, \ldots, N-1$ **do**
14: $z_t^j = y_t^j + \gamma(y_t^j - y_t^{j-1})$
15: $y_t^{j+1} = z_t^j - \alpha \nabla_y G(x_t, z_t^j; \pi_t^j)$, where $\pi_t^j \sim \mathcal{D}_g$
16: **end for**
17: $y_{t+1} = y_t^{N+1}$
18: **else**
19: $y_{t+1} = y_t$
20: **end if**
21: $\hat{y}_{t+1} = (1-\tau)\hat{y}_t + \tau y_{t+1}$ # Averaging
22: # Upper-Level: Normalized Stochastic Gradient Descent with Recursive Momentum
23: $m_t = \beta m_{t-1} + (1-\beta)\bar{\nabla} f(x_t, \hat{y}_t; \bar{\xi}_t) + \beta(\bar{\nabla} f(x_t, \hat{y}_t; \bar{\xi}_t) - \bar{\nabla} f(x_{t-1}, \hat{y}_{t-1}; \bar{\xi}_t))$ if $t \geq 1$ else $m_0 = \bar{\nabla} f(x_0, \hat{y}_0; \bar{\xi}_0)$
24: $x_{t+1} = x_t - \eta \frac{m_t}{\|m_t\|}$
25: **end for**

(59)*, and* (60)*) as*

$$\alpha^{\text{init}} = \widetilde{\Theta}(\epsilon^4), \quad \alpha = \widetilde{\Theta}(\epsilon^2), \quad 1-\beta = \widetilde{\Theta}(\epsilon^2), \quad \eta = \widetilde{\Theta}(\epsilon^2), \quad \tau = \widetilde{\Theta}(\epsilon), \quad \gamma = O(1),$$
$$T_0 = \widetilde{O}(\epsilon^{-2}), \quad I = \widetilde{O}(\epsilon^{-1}), \quad N = \widetilde{O}(\epsilon^{-1}), \quad Q = \widetilde{O}(1), \quad S = \widetilde{O}(1).$$

Then with probability at least $1 - 2\delta$ *over the randomness in* $\sigma(\mathcal{F}^{\text{init}} \cup \widetilde{\mathcal{F}}_T^1)$ *(for Option I) or* $\sigma(\mathcal{F}^{\text{init}} \cup (\cup_{t \leq T} \widetilde{\mathcal{F}}_t^2))$ *(for Option II), Algorithm 2 guarantees* $\frac{1}{T}\sum_{t=1}^{T} \mathbb{E}\|\nabla \Phi(x_t)\| \leq 20\epsilon$ *within* $T = \frac{4d_0}{\eta\epsilon} = \widetilde{O}(\epsilon^{-3})$ *iterations, where* $d_0 := \Phi(x_0) - \inf_x \Phi(x)$ *and the expectation is taken over the randomness over* $\mathcal{F}_T$*. For Option I, it requires* $T_0 + SQT = \widetilde{O}(\epsilon^{-3})$ *oracle calls of stochastic gradient or Hessian/Jacobian vector product. For Option II, it requires* $T_0 + \frac{NT}{I} + SQT = \widetilde{O}(\epsilon^{-3})$ *oracle calls of stochastic gradient or Hessian/Jacobian vector product.*

Remark: Theorem 4.1 established an improved $\widetilde{O}(\epsilon^{-3})$ oracle complexity for finding an ϵ-stationary point when the lower-level standard deviation $\sigma_{g,1} = O(\sqrt{\epsilon})$. This complexity result strictly improves the $\widetilde{O}(\epsilon^{-4})$ obtained by [38, 32] when the upper-level function is nonconvex and unbounded smooth. This complexity result also matches that in the single-level unbounded smooth setting [56] and is nearly optimal in terms of the dependency on ϵ [2]. The full statement of Theorem 4.1 is included in Theorem E.2.

4.3 Proof Sketch

In this section, we provide a roadmap of proving Theorem 4.1 and the main steps. The detailed proofs can be found in Appendix D and E. The key idea is to prove two things: (1) the lower-level iterate is very close to the optimal lower-level variable at every iteration; (2) two consecutive iterates of the lower-level iterates are close to each other. In particular, define $y_t^* = y^*(x_t)$, and we aim to prove that $\|\hat{y}_t - y_t^*\| \leq O(\epsilon)$ and $\|\hat{y}_{t+1} - \hat{y}_t\| \leq O(\epsilon^2)$ for every t. These two requirements are essential to control the hypergradient estimation error (i.e., $\|m_t - \nabla \Phi(x_t)\|$) caused by inaccurate estimate of the lower-level problem. Lemma 4.7 provides the guarantee for the lower-level problem, and Lemma 4.8

characterizes the hypergradient estimation error. Equipped with these two lemmas, we can adapt the momentum-based variance reduction techniques [18, 56] to the upper-level problem and prove the main theorem.

The main technical contribution of this paper is to provide a general framework for proving the convergence of SNAG under distributional drift in Section 4.3.1, which can be leveraged as a tool to control the lower-level error in bilevel optimization and derive the Lemma 4.7, as illustrated in Section 4.3.2. In particular, we can regard the change of the upper-level variable x at each iteration as the distributional drift for the lower-level problem: the drift is small due to the normalization operator of the upper-level update rule and also the Lipschitzness of $y^*(x)$. Once we have the general lemma for tracking the minimizer for any fixed distributional drift over time, this lemma can be applied to our algorithm analysis and establish guarantees for the bilevel problem.

4.3.1 Stochastic Nesterov Accelerated Gradient Descent under Distributional Drift

In this section, we study the sequences of stochastic optimization problems $\min_{w\in\mathbb{R}^d} \phi_t(w)$ indexed by time $t \in \mathbb{N}$. We denote the minimizer and the minimal value of ϕ_t as w_t^* and ϕ_t^*, and we define the *minimizer drift* at time t to be $\Delta_t := \|w_t^* - w_{t+1}^*\|$. With a slight abuse of notation [3], we consider the SNAG algorithm applied to the sequence $\{\phi_t\}_{t=1}^T$, where T is the total number of iterations:

$$\begin{aligned} z_t &= w_t + \gamma(w_t - w_{t-1}) \\ w_{t+1} &= w_t + \gamma(w_t - w_{t-1}) - \alpha g_t, \end{aligned} \tag{3}$$

where $g_t = \nabla\phi_t(z_t;\xi_t)$ is the stochastic gradient evaluated at z_t with random sample ξ_t. Define $\varepsilon_t = g_t - \nabla\phi_t(z_t)$ as the stochastic gradient noise at t-th iteration. Define $\mathcal{H}_t = \sigma(\xi_1, \dots, \xi_{t-1})$ as the filtration, which is the σ-algebra generated by all random variables until t-th iteration. We make the following assumption, which is the same as Assumption 3 in [20] for high probability analysis.

Assumption 4.2. *Function $\phi_t : \mathbb{R}^d \to \mathbb{R}$ is μ-strongly convex and L-smooth for constants $\mu, L > 0$. Also, there exists constants $\Delta, \sigma > 0$ such that the drift Δ_t^2 is sub-exponential conditioned on $\mathcal{H}_t$ with parameter Δ^2 and the noise ε_t is norm sub-Gaussian conditioned on $\mathcal{H}_t$ with parameter $\sigma/2$.*

Lemma 4.3. *Suppose Assumption 4.2 holds and let $\{w_t\}$ be the iterates produced by the update rule* (3) *with constant learning rate $\alpha \le 1/25L$, and set $\gamma = \frac{1-\sqrt{\mu\alpha}}{1+\sqrt{\mu\alpha}}$. Define $\theta_t = [(w_t - w_t^*)^\top, (w_{t-1} - w_t^*)^\top]^\top \in \mathbb{R}^{2d}$, and the potential function V_t as*

$$V_t = \theta_t^\top \mathbf{P}\theta_t + \phi_t(w_t) - \phi_t(w_t^*), \quad \textit{where} \quad \mathbf{P} = \frac{1}{2\alpha}\begin{bmatrix} 1 & \sqrt{\mu\alpha}-1 \\ \sqrt{\mu\alpha}-1 & (1-\sqrt{\mu\alpha})^2 \end{bmatrix} \otimes \mathbf{I}_d.$$

Then for any given $\delta \in (0,1)$ and all $t \ge 0$, the following holds with probability at least $1-\delta$ over the randomness in $\mathcal{H}_t$ (here e denotes the base of natural logarithms):

(i) (With drift) Let $\phi_t(w) := \frac{\mu}{2}\|w - w_t^*\|^2$, then $V_t \le \left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^t V_0 + \left(\frac{5\sqrt{\alpha}\sigma^2}{\sqrt{\mu}} + \frac{80\Delta^2}{\alpha}\right)\ln\frac{eT}{\delta}$.

(ii) (Without drift) Let $\phi_t(w) \equiv \phi(w)$ be any general strongly convex functions with $\Delta = 0$, then $V_t \le \left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^t V_0 + \frac{5\sqrt{\alpha}\sigma^2}{\sqrt{\mu}}\ln\frac{eT}{\delta}$.

Remark: When $\{\phi_t\}_{t=1}^T$ is a sequence of quadratic functions with moving minimizers, Lemma 4.3 provides a high probability tracking guarantee for SNAG with distributional drift, which is useful to provide guarantees for Option I in Algorithm 2. Note that this guarantee strictly improves the guarantee of stochastic gradient descent with distributional drift (e.g., [20, Theorem 6]) *in the small stochastic gradient noise regime* and therefore is of independent interest. In particular, for small α, the decaying factor in the first term is improved from $1 - \frac{\mu\alpha}{2}$ to $1 - \frac{\sqrt{\mu\alpha}}{4}$, the drift term is improved from $\frac{\Delta^2}{\mu\alpha^2}$ to $\frac{\Delta^2}{\alpha}$, and the variance term becomes a bit worse (from $\alpha\sigma^2$ to $\frac{\sqrt{\alpha}\sigma^2}{\sqrt{\mu}}$). When σ is small enough, the variance term becomes insignificant compared with the drift term, then Lemma 4.3 provides an improved convergence rate with high probability. To the best of our knowledge, such an improved guarantee for SNAG with distributional drift is first shown in this work. When there is no drift, Lemma 4.3 also provides a high probability guarantee for SNAG. It holds for any smooth and strongly convex function ϕ, and it is useful to provide guarantees for Option II of Algorithm 2.

[3] The notation in Section 4.3.1 is independent of that in other sections, although there may be incidental overlaps in terminology.

4.3.2 Application of Stochastic Nesterov Accelerated Gradient to Bilevel Optimization

Inspired by [38, 32], we can regard $\phi_t(\cdot)$ as $\phi_t(\cdot) := g(x_t, \cdot)$ in the bilevel setting, and then we have $\Delta_t = \eta l_{g,1}/\mu$ for every t due to the upper-level update rule and the Lipschitzness of $y^*(x)$. Therefore we can focus on the high probability analysis on the lower-level variable without worrying about the randomness from the upper-level. Throughout, we assume Assumption 3.1, 3.2, 3.3 and 3.4 hold. In addition, the failure probability $\delta \in (0, 1)$ and $\epsilon > 0$ are chosen in the same way as in Theorem 4.1.

Lemma 4.4 (Warm-start)**.** *Let $\{y_t^{\text{init}}\}$ be the iterates produced by line 2 of Algorithm 2. Set $\alpha^{\text{init}} = \widetilde{\Theta}(\epsilon^4)$, $\sigma_{g,1} = (\mu\alpha)^{1/4}\tilde{\sigma}_{g,1}$, and $\phi_t(y) \equiv g(x_0, y)$. Then $\|y_{T_0}^{\text{init}} - y_0^*\| \leq \sqrt{\frac{\mu\alpha}{32}}\frac{\epsilon}{L_0}$ holds with probability at least $1-\delta$ over the randomness in $\widetilde{\mathcal{F}}^{\text{init}}$ (we denote this event as $\mathcal{E}_{\text{init}}$) in $T_0 = \widetilde{O}(\epsilon^{-2})$ iterations.*

Remark: Lemma 4.4 shows that for fixed initialization x_0, running SNAG for at most $T_0 = \widetilde{O}(\epsilon^{-2})$ iterations can guarantee that the Euclidean distance between the lower-level variable $y_{T_0}^{\text{init}}$ and the optimal solution $y^*(x_0)$ is at most $O(\epsilon)$, with high probability.

Lemma 4.5 (Option I)**.** *Under event $\mathcal{E}_{\text{init}}$, let $\{y_t\}$ be the iterates produced by Option I. Set $\alpha = \widetilde{\Theta}(\epsilon^2)$, $\sigma_{g,1} = (\mu\alpha)^{1/4}\tilde{\sigma}_{g,1}$, and $\phi_t(y) = g(x_t, y) = \frac{\mu}{2}\|y - y_t^*\|^2$. Then for any $t \in [T]$, Algorithm 2 guarantees with probability at least $1-\delta$ over the randomness in $\widetilde{\mathcal{F}}_T^1$ (we denote this event as $\mathcal{E}_y^1$) that $\|y_t - y_t^*\| \leq \epsilon/2L_0$.*

Lemma 4.6 (Option II)**.** *Under event $\mathcal{E}_{\text{init}}$, let $\{y_t\}$ be the iterates produced by Option II. Set $\alpha = \widetilde{\Theta}(\epsilon^2)$, $N = \widetilde{O}(\epsilon^{-1})$, $I = \widetilde{O}(\epsilon^{-1})$, $\sigma_{g,1} = (\mu\alpha)^{1/4}\tilde{\sigma}_{g,1}$, and $\phi_t(y) = g(x_t, y)$ when t is a multiple of I (i.e., x_t is fixed for each update round of Option II so g can be general functions). Then for any $t \in [T]$, Algorithm 2 guarantees with probability at least $1-\delta$ over the randomness in $\sigma(\cup_{t\leq T}\widetilde{\mathcal{F}}_t^2)$ (we denote this event as $\mathcal{E}_y^2$) that $\|y_t - y_t^*\| \leq \epsilon/L_0$.*

Remark: Lemma 4.5 and Lemma 4.6 show that, under event $\mathcal{E}_{\text{init}}$ and both option I and option II, the algorithm guarantees that each iterate y_t is $O(\epsilon)$-close to the the optimal lower-level variable y_t^* at every iteration t with high probability.

Lemma 4.7 (Averaging)**.** *Under event $\mathcal{E}_{\text{init}} \cap \mathcal{E}_y^1$ (Option I) or $\mathcal{E}_{\text{init}} \cap \mathcal{E}_y^2$ (Option II), set $\tau = \sqrt{\mu\alpha}$ in the averaging step (line 21 of Algorithm 2). Then for any $t \geq 0$ we have $\|\hat{y}_t - y_t^*\| \leq \frac{2\epsilon}{L_0}$ and $\|\hat{y}_{t+1} - \hat{y}_t\| \leq \frac{\mu\epsilon^2}{24L_0^2\sigma_{g,1}} =: \vartheta$.*

Remark: Lemma 4.7 shows that after performing averaging operations over the sequence $\{y_t\}_{t=1}^T$, the averaged sequence enjoys stronger guarantees. First, each averaged iterate $\hat{y}_t$ is still $O(\epsilon)$-close to the optimal lower-level variable y_t^*; Second, two consecutive averaged iterates (i.e., $\hat{y}_t$ and $\hat{y}_{t+1}$) is $O(\epsilon^2)$-close to each other. The stronger guarantees are crucial to control the hypergradient estimation error as described in Lemma 4.8.

Lemma 4.8. *Under event $\mathcal{E}_{\text{init}} \cap \mathcal{E}_y^1$ (Option I) or $\mathcal{E}_{\text{init}} \cap \mathcal{E}_y^2$ (Option II), define $\epsilon_t = m_t - \mathbb{E}_t[\bar{\nabla} f(x_t, \hat{y}_t; \bar{\xi}_t)]$, then we have the following averaged cumulative error bound:*

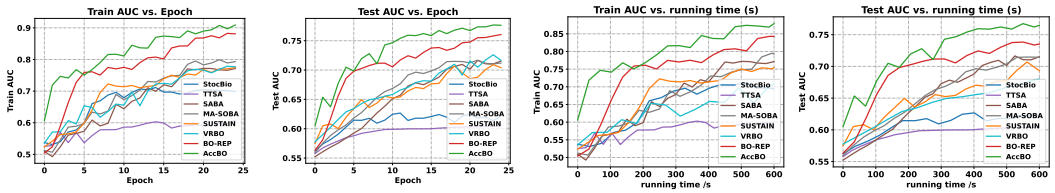
$$\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\epsilon_t\| \leq \frac{\bar{\sigma}}{T(1-\beta)} + \sqrt{1-\beta}\bar{\sigma} + \frac{\bar{L}_0}{\sqrt{1-\beta}}\sqrt{\frac{2(\eta^2+\vartheta^2)}{S}} + \bar{L}_1\sqrt{\frac{2(\eta^2+\vartheta^2)}{S(1-\beta)}}\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\nabla\Phi(x_t)\|,$$

where S denotes the batch size, and $\bar{\sigma}, \bar{L}_0, \bar{L}_1$ are defined in Lemmas B.4 and B.6.

Remark: Lemma 4.8 characterizes the upper-level hypergradient estimation error under the good event that the lower-level error can be controlled. One can choose hyperparameters appropriately such that the cumulative error (i.e., LHS) grows only sublinearly in terms of T, which is important for establishing the fast convergence of our algorithm.

5 Experiments

Deep AUC Maximization with Recurrent Neural Networks. AUC (Area Under the ROC Curve) [36] is a critical metric in evaluating the performance of binary classification models. It measures the ability of the model to distinguish between positive and negative classes, and



(a) Training AUC (b) Test AUC (c) Training AUC vs. running time (d) Test AUC vs. running time

Figure 1: Results of bilevel optimization on deep AUC maximization. Figure (a), (b) are the results over epochs, and Figure (c), (d) are the results over running time.

it is defined as the probability that the prediction score of a positive example is higher than that is a negative example [35]. Deep AUC maximization [53, 72] can be formulated as a min-max optimization problem [53]: $\min_{\boldsymbol{w}\in\mathbb{R}^d,(a,b)\in\mathbb{R}^2} \max_{\alpha\in\mathbb{R}} f(\boldsymbol{w},a,b,\alpha) := \mathbb{E}_{\boldsymbol{z}}[F(\boldsymbol{w},a,b,\alpha;\boldsymbol{z})]$, where $F(\boldsymbol{w},a,b,\alpha;\boldsymbol{z}) = (1-r)(h(\boldsymbol{w};\boldsymbol{x})-a)^2\mathbb{I}_{[c=1]} + r(h(\boldsymbol{w};\boldsymbol{x})-b)^2\mathbb{I}_{[c=-1]} + 2(1+\alpha)(rh(\boldsymbol{w};\boldsymbol{x})\mathbb{I}_{[c=-1]} - (1-r)h(\boldsymbol{w};\boldsymbol{x})\mathbb{I}_{[c=1]}) - r(1-r)\alpha^2$, $\boldsymbol{w}$ denotes the model parameter, $\boldsymbol{z}=(\boldsymbol{x},c)$ is the random data sample ($\boldsymbol{x}$ denote the feature vector and $c\in\{+1,-1\}$ denotes the label), $h(\boldsymbol{w},\boldsymbol{x})$ is the score function defined by a neural network, and $r=\Pr(c=1)$ denotes the ratio of positive samples in the population. This min-max formulation is an special case of the bilevel problem with $g=-f$ in (1), which can be reformulated as the following:

$$\min_{\boldsymbol{w}\in\mathbb{R}^d,(a,b)\in\mathbb{R}^2} \mathbb{E}_{\boldsymbol{z}}[F(\boldsymbol{w},a,b,\alpha^*(\boldsymbol{w},a,b);\boldsymbol{z})] \quad \text{s.t.,} \quad \alpha^*(\boldsymbol{w},a,b)\in\arg\min_{\alpha\in\mathbb{R}} -\mathbb{E}_{\boldsymbol{z}}[F(\boldsymbol{w},a,b,\alpha;\boldsymbol{z})] \tag{4}$$

where $(\boldsymbol{w},a,b)$ denotes the upper-level variable, and α denotes the lower-level variable. In this case, the lower-level is a quadratic function in terms of α and is strongly convex, and the upper-level function is non-convex function with potential unbounded smoothness when using a recurrent neural network as the predictive model.

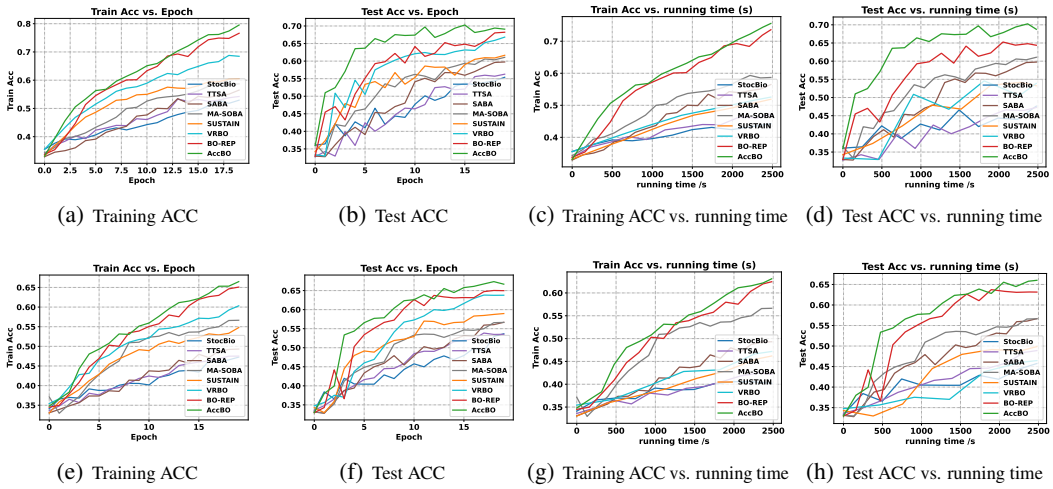
We aim to perform imbalanced text classification task and maximize the AUC metric. The Deep AUC maximization experiment is performed on imbalanced Sentiment140 [31] dataset (under the license of CC BY 4.0), which is a binary text classification task. Specifically, we follow [73] to make training set imbalanced with a pre-defined imbalanced ratio (r), and leave the test set unchanged. Given r, we randomly discard the positive samples (with label 1) in original training set until the portion of positive samples equals to r. The imbalance ratio r is set to 0.2 in our experiment, which means only 20% data is positive in the training set. We use a two-layer recurrent neural network with input dimension=300, hidden dimension=4096, and output dimension=2 for the model prediction.

We compare with some bilevel optimization baselines, including StocBio [44], TTSA [41], SABA [21], MA-SOBA [12], SUSTAIN [46], VRBO [71] and BO-REP [38]. We show the training and test AUC result with 25 epochs in (a) (b) of Figure 1 and running time in (c), (d) of Figure 1. Our algorithm AccBO achieves highest AUC score among all the baselines over epochs and running time. The running time figure shows AccBO converges to a good result faster than other baselines. The detailed parameter tuning and selection are included in Appendix G.

Data Hypercleaning. The Data hypercleaning task tries to learn a set of weights $\boldsymbol{\lambda}$ for the corrupted training data $\mathcal{D}_{tr}$, such that the model trained on the weighted corrupted training set can achieve good performance on the clean validation set $\mathcal{D}_{val}$, where the corrupted training set $\mathcal{D}_{tr} := \{\boldsymbol{x}_i, \bar{y}_i\}$ and the label $\bar{y}_i$ is randomly flipped to one of other labels with probability $0<p<1$. The data hyper-cleaning can be formulated as a bilevel optimization problem,

$$\min_{\boldsymbol{\lambda}} \frac{1}{|\mathcal{D}_{\text{val}}|}\sum_{\xi\in\mathcal{D}_{\text{val}}} \mathcal{L}(\boldsymbol{w}^*(\boldsymbol{\lambda});\xi), \text{ s.t. } \boldsymbol{w}^*(\boldsymbol{\lambda})\in\arg\min_{\boldsymbol{w}} \frac{1}{|\mathcal{D}_{\text{tr}}|}\sum_{\zeta_i\in\mathcal{D}_{\text{tr}}} \sigma(\lambda_i)\mathcal{L}(\boldsymbol{w};\zeta_i) + c\|\boldsymbol{w}\|^2, \tag{5}$$

where $\boldsymbol{w}$ is the model parameter of a neural network, and $\sigma(x)=\frac{1}{1+e^{-x}}$ is the sigmoid function. We perform bilevel optimization algorithms on the noisy text classification dataset Stanford Natural Language Inference (SNLI) [8] (under the license of CC BY 4.0) with a three-layer recurrent neural network with input dimension=300, hidden dimension=4096, and output dimension=3 for the label prediction. Each of sentence-pairs manually labeled as entailment, contradiction, and neutral.



(a) Training ACC (b) Test ACC (c) Training ACC vs. running time (d) Test ACC vs. running time

(e) Training ACC (f) Test ACC (g) Training ACC vs. running time (h) Test ACC vs. running time

Figure 2: Results of bilevel optimization on data hyper-cleaning with $p = 0.1$. Figure (a), (b), (c), (d) are the results with noise rate $p = 0.1$ where (a), (b) are the results over epochs, and Figure (c), (d) are the results over running time. Figure (e), (f), (g), (h) are the results with noise rate $p = 0.2$.

Specifically, the label of each training data is randomly flipped to one of the other two labels with probability p. We set $p = 0.1$ and $p = 0.2$ in the experiments, respectively. We compare all the baselines used in the deep AUC maximization experiment. Different from the formulation (4) for the deep AUC maximization, the lower-level function in (5) is not quadratic function of the lower-level variable. Therefore we choose Option II in Algorithm 2, i.e., periodic updates for the lower-level variable. The results are presented in Figure 2 ($p = 0.1$ and $p = 0.2$). Our algorithm AccBO exhibits the highest classification accuracy on training and test set among all the bilevel baselines, and also shows a high runtime efficiency. More detailed parameter tuning and selection can be found in Appendix G. All the experiments are run on the device of NVIDIA A6000 (48GB memory) GPU and AMD EPYC 7513 32-Core CPU.

6 Conclusion

In this paper, we propose a new algorithm named AccBO for solving bilevel optimization problems where the upper-level is nonconvex and unbounded smooth and the lower-level problem is strongly convex. The algorithm achieved $\widetilde{O}(\epsilon^{-3})$ oracle complexity for finding an ϵ-stationary point when the lower-level stochastic gradient variance is $O(\epsilon)$, which matches the rate of the state-of-the-art single-level relaxed smooth optimization [56] and is nearly optimal in terms of dependency on ϵ [2].

Limitations. There are two limitations of our work. One limitation of our work is that the convergence analysis for the Option I of our algorithm relies on the lower-level problem being a quadratic function: only under this case the algorithm becomes a single-loop procedure. Another limitation is that we require the lower-level stochastic gradient has variance $O(\epsilon)$. It remains unclear how to design single-loop algorithms for more general lower-level strongly convex functions and get rid of the small stochastic gradient variance assumption for the lower-level variable.

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References

[1] G Anandalingam and DJ White. A solution method for the linear static stackelberg problem using penalty functions. *IEEE Transactions on automatic control*, 35(10):1170–1173, 1990.

[2] Yossi Arjevani, Yair Carmon, John C Duchi, Dylan J Foster, Nathan Srebro, and Blake Woodworth. Lower bounds for non-convex stochastic optimization. *Mathematical Programming*, 199 (1-2):165–214, 2023.

[3] Mahmoud Assran and Michael Rabbat. On the convergence of nesterov's accelerated gradient method in stochastic settings. *arXiv preprint arXiv:2002.12414*, 2020.

[4] Necdet Serhat Aybat, Alireza Fallah, Mert Gurbuzbalaban, and Asuman Ozdaglar. A universally optimal multistage accelerated stochastic gradient method. *Advances in neural information processing systems*, 32, 2019.

[5] Necdet Serhat Aybat, Alireza Fallah, Mert Gurbuzbalaban, and Asuman Ozdaglar. Robust accelerated gradient methods for smooth strongly convex functions. *SIAM Journal on Optimization*, 30(1):717–751, 2020.

[6] Omar Besbes, Yonatan Gur, and Assaf Zeevi. Non-stationary stochastic optimization. *Operations research*, 63(5):1227–1244, 2015.

[7] Zalán Borsos, Mojmir Mutny, and Andreas Krause. Coresets via bilevel optimization for continual learning and streaming. *Advances in neural information processing systems*, 33: 14879–14890, 2020.

[8] Samuel R Bowman, Gabor Angeli, Christopher Potts, and Christopher D Manning. A large annotated corpus for learning natural language inference. *arXiv preprint arXiv:1508.05326*, 2015.

[9] Jerome Bracken and James T McGill. Mathematical programs with optimization problems in the constraints. *Operations research*, 21(1):37–44, 1973.

[10] Lesi Chen, Jing Xu, and Jingzhao Zhang. On bilevel optimization without lower-level strong convexity. *arXiv preprint arXiv:2301.00712*, 2023.

[11] Tianyi Chen, Yuejiao Sun, and Wotao Yin. Closing the gap: Tighter analysis of alternating stochastic gradient methods for bilevel problems. *Advances in Neural Information Processing Systems*, 34:25294–25307, 2021.

[12] Xuxing Chen, Tesi Xiao, and Krishnakumar Balasubramanian. Optimal algorithms for stochastic bilevel optimization under relaxed smoothness conditions. *arXiv preprint arXiv:2306.12067*, 2023.

[13] You-Lin Chen, Sen Na, and Mladen Kolar. Convergence analysis of accelerated stochastic gradient descent under the growth condition. *Mathematics of Operations Research*, 2023.

[14] Ziyi Chen, Yi Zhou, Yingbin Liang, and Zhaosong Lu. Generalized-smooth nonconvex optimization is as efficient as smooth nonconvex optimization. *arXiv preprint arXiv:2303.02854*, 2023.

[15] Michael Crawshaw, Mingrui Liu, Francesco Orabona, Wei Zhang, and Zhenxun Zhuang. Robustness to unbounded smoothness of generalized signsgd. *Advances in neural information processing systems*, 2022.

[16] Michael Crawshaw, Yajie Bao, and Mingrui Liu. Episode: Episodic gradient clipping with periodic resampled corrections for federated learning with heterogeneous data. In *The Eleventh International Conference on Learning Representations*, 2023.

[17] Michael Crawshaw, Yajie Bao, and Mingrui Liu. Federated learning with client subsampling, data heterogeneity, and unbounded smoothness: A new algorithm and lower bounds. In *Thirty-seventh Conference on Neural Information Processing Systems*, 2023.

[18] Ashok Cutkosky and Francesco Orabona. Momentum-based variance reduction in non-convex sgd. *Advances in neural information processing systems*, 32, 2019.

[19] Joshua Cutler, Dmitriy Drusvyatskiy, and Zaid Harchaoui. Stochastic optimization under time drift: iterate averaging, step-decay schedules, and high probability guarantees. *Advances in neural information processing systems*, 34:11859–11869, 2021.

[20] Joshua Cutler, Dmitriy Drusvyatskiy, and Zaid Harchaoui. Stochastic optimization under distributional drift. *Journal of Machine Learning Research*, 24(147):1–56, 2023.

[21] Mathieu Dagréou, Pierre Ablin, Samuel Vaiter, and Thomas Moreau. A framework for bilevel optimization that enables stochastic and global variance reduction algorithms. *Advances in Neural Information Processing Systems*, 35:26698–26710, 2022.

[22] Jeffrey L Elman. Finding structure in time. *Cognitive science*, 14(2):179–211, 1990.

[23] Cong Fang, Chris Junchi Li, Zhouchen Lin, and Tong Zhang. Spider: Near-optimal non-convex optimization via stochastic path-integrated differential estimator. *Advances in neural information processing systems*, 31, 2018.

[24] Matthew Faw, Litu Rout, Constantine Caramanis, and Sanjay Shakkottai. Beyond uniform smoothness: A stopped analysis of adaptive sgd. *arXiv preprint arXiv:2302.06570*, 2023.

[25] Matthias Feurer and Frank Hutter. Hyperparameter optimization. In *Automated Machine Learning*, pages 3–33. Springer, Cham, 2019.

[26] Chelsea Finn, Pieter Abbeel, and Sergey Levine. Model-agnostic meta-learning for fast adaptation of deep networks. In *International conference on machine learning*, pages 1126–1135. PMLR, 2017.

[27] Luca Franceschi, Paolo Frasconi, Saverio Salzo, Riccardo Grazzi, and Massimiliano Pontil. Bilevel programming for hyperparameter optimization and meta-learning. In *International conference on machine learning*, pages 1568–1577. PMLR, 2018.

[28] Saeed Ghadimi and Guanghui Lan. Stochastic first-and zeroth-order methods for nonconvex stochastic programming. *SIAM Journal on Optimization*, 23(4):2341–2368, 2013.

[29] Saeed Ghadimi and Guanghui Lan. Accelerated gradient methods for nonconvex nonlinear and stochastic programming. *Mathematical Programming*, 156(1-2):59–99, 2016.

[30] Saeed Ghadimi and Mengdi Wang. Approximation methods for bilevel programming. *arXiv preprint arXiv:1802.02246*, 2018.

[31] Alec Go, Richa Bhayani, and Lei Huang. Twitter sentiment classification using distant supervision. *CS224N project report, Stanford*, 1(12):2009, 2009.

[32] Xiaochuan Gong, Jie Hao, and Mingrui Liu. A nearly optimal single loop algorithm for stochastic bilevel optimization under unbounded smoothness. In *Forty-first International Conference on Machine Learning*, 2024.

[33] Riccardo Grazzi, Massimiliano Pontil, and Saverio Salzo. Bilevel optimization with a lower-level contraction: Optimal sample complexity without warm-start. *arXiv preprint arXiv:2202.03397*, 2022.

[34] Zhishuai Guo, Quanqi Hu, Lijun Zhang, and Tianbao Yang. Randomized stochastic variance-reduced methods for multi-task stochastic bilevel optimization. *arXiv preprint arXiv:2105.02266*, 2021.

[35] James A Hanley and Barbara J McNeil. The meaning and use of the area under a receiver operating characteristic (roc) curve. *Radiology*, 143(1):29–36, 1982.

[36] James A Hanley and Barbara J McNeil. A method of comparing the areas under receiver operating characteristic curves derived from the same cases. *Radiology*, 148(3):839–843, 1983.

[37] Jie Hao, Kaiyi Ji, and Mingrui Liu. Bilevel coreset selection in continual learning: A new formulation and algorithm. *Advances in Neural Information Processing Systems*, 36, 2023.

[38] Jie Hao, Xiaochuan Gong, and Mingrui Liu. Bilevel optimization under unbounded smoothness: A new algorithm and convergence analysis. In *The Twelfth International Conference on Learning Representations*, 2024.

[39] Elad Hazan and Satyen Kale. Beyond the regret minimization barrier: optimal algorithms for stochastic strongly-convex optimization. *Journal of Machine Learning Research*, 15(1): 2489–2512, 2014.

[40] Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. *Neural computation*, 9(8): 1735–1780, 1997.

[41] Mingyi Hong, Hoi-To Wai, Zhaoran Wang, and Zhuoran Yang. A two-timescale stochastic algorithm framework for bilevel optimization: Complexity analysis and application to actor-critic. *SIAM Journal on Optimization*, 33(1):147–180, 2023.

[42] Bin Hu and Laurent Lessard. Dissipativity theory for nesterov's accelerated method. In *International Conference on Machine Learning*, pages 1549–1557. PMLR, 2017.

[43] Quanqi Hu, Zi-Hao Qiu, Zhishuai Guo, Lijun Zhang, and Tianbao Yang. Blockwise stochastic variance-reduced methods with parallel speedup for multi-block bilevel optimization. In *International Conference on Machine Learning*, pages 13550–13583. PMLR, 2023.

[44] Kaiyi Ji, Junjie Yang, and Yingbin Liang. Bilevel optimization: Convergence analysis and enhanced design. In *International conference on machine learning*, pages 4882–4892. PMLR, 2021.

[45] Jikai Jin, Bohang Zhang, Haiyang Wang, and Liwei Wang. Non-convex distributionally robust optimization: Non-asymptotic analysis. *Advances in Neural Information Processing Systems*, 34:2771–2782, 2021.

[46] Prashant Khanduri, Siliang Zeng, Mingyi Hong, Hoi-To Wai, Zhaoran Wang, and Zhuoran Yang. A near-optimal algorithm for stochastic bilevel optimization via double-momentum. *Advances in Neural Information Processing Systems (NeurIPS)*, 34:30271–30283, 2021.

[47] Vijay Konda and John Tsitsiklis. Actor-critic algorithms. *Advances in neural information processing systems*, 12, 1999.

[48] Jeongyeol Kwon, Dohyun Kwon, Stephen Wright, and Robert D Nowak. A fully first-order method for stochastic bilevel optimization. In *International Conference on Machine Learning*, pages 18083–18113. PMLR, 2023.

[49] Jeongyeol Kwon, Dohyun Kwon, Steve Wright, and Robert Nowak. On penalty methods for nonconvex bilevel optimization and first-order stochastic approximation. *arXiv preprint arXiv:2309.01753*, 2023.

[50] Guanghui Lan. An optimal method for stochastic composite optimization. *Mathematical Programming*, 133(1-2):365–397, 2012.

[51] Haochuan Li, Ali Jadbabaie, and Alexander Rakhlin. Convergence of adam under relaxed assumptions. *arXiv preprint arXiv:2304.13972*, 2023.

[52] Bo Liu, Mao Ye, Stephen Wright, Peter Stone, and Qiang Liu. Bome! bilevel optimization made easy: A simple first-order approach. *Advances in Neural Information Processing Systems*, 35:17248–17262, 2022.

[53] Mingrui Liu, Zhuoning Yuan, Yiming Ying, and Tianbao Yang. Stochastic auc maximization with deep neural networks. *ICLR*, 2020.

[54] Mingrui Liu, Zhenxun Zhuang, Yunwen Lei, and Chunyang Liao. A communication-efficient distributed gradient clipping algorithm for training deep neural networks. *Advances in Neural Information Processing Systems*, 35:26204–26217, 2022.

[55] Risheng Liu, Pan Mu, Xiaoming Yuan, Shangzhi Zeng, and Jin Zhang. A generic first-order algorithmic framework for bi-level programming beyond lower-level singleton. In *International Conference on Machine Learning*, pages 6305–6315. PMLR, 2020.

[56] Zijian Liu, Srikanth Jagabathula, and Zhengyuan Zhou. Near-optimal non-convex stochastic optimization under generalized smoothness. *arXiv preprint arXiv:2302.06032*, 2023.

[57] Liam Madden, Stephen Becker, and Emiliano Dall'Anese. Bounds for the tracking error of first-order online optimization methods. *Journal of Optimization Theory and Applications*, 189: 437–457, 2021.

[58] Yurii Nesterov. A method of solving a convex programming problem with convergence rate o (1/k2). In *Soviet Mathematics Doklady*, volume 27, pages 372–376, 1983.

[59] Aravind Rajeswaran, Chelsea Finn, Sham M Kakade, and Sergey Levine. Meta-learning with implicit gradients. In *Advances in Neural Information Processing Systems (NeurIPS)*, pages 113–124, 2019.

[60] Amirhossein Reisizadeh, Haochuan Li, Subhro Das, and Ali Jadbabaie. Variance-reduced clipping for non-convex optimization. *arXiv preprint arXiv:2303.00883*, 2023.

[61] Shoham Sabach and Shimrit Shtern. A first order method for solving convex bilevel optimization problems. *SIAM Journal on Optimization*, 27(2):640–660, 2017.

[62] Han Shen and Tianyi Chen. On penalty-based bilevel gradient descent method. *arXiv preprint arXiv:2302.05185*, 2023.

[63] Daouda Sow, Kaiyi Ji, Ziwei Guan, and Yingbin Liang. A constrained optimization approach to bilevel optimization with multiple inner minima. *arXiv preprint arXiv:2203.01123*, 2022.

[64] Quoc Tran-Dinh, Nhan H Pham, Dzung T Phan, and Lam M Nguyen. Hybrid stochastic gradient descent algorithms for stochastic nonconvex optimization. *arXiv preprint arXiv:1905.05920*, 2019.

[65] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in neural information processing systems*, 30, 2017.

[66] Sharan Vaswani, Benjamin Dubois-Taine, and Reza Babanezhad. Towards noise-adaptive, problem-adaptive (accelerated) stochastic gradient descent. In *International conference on machine learning*, pages 22015–22059. PMLR, 2022.

[67] Luis Vicente, Gilles Savard, and Joaquim Júdice. Descent approaches for quadratic bilevel programming. *Journal of optimization theory and applications*, 81(2):379–399, 1994.

[68] Bohan Wang, Huishuai Zhang, Zhiming Ma, and Wei Chen. Convergence of adagrad for non-convex objectives: Simple proofs and relaxed assumptions. In *The Thirty Sixth Annual Conference on Learning Theory*, pages 161–190. PMLR, 2023.

[69] Douglas J White and G Anandalingam. A penalty function approach for solving bi-level linear programs. *Journal of Global Optimization*, 3:397–419, 1993.

[70] Craig Wilson, Venugopal V Veeravalli, and Angelia Nedić. Adaptive sequential stochastic optimization. *IEEE Transactions on Automatic Control*, 64(2):496–509, 2018.

[71] Junjie Yang, Kaiyi Ji, and Yingbin Liang. Provably faster algorithms for bilevel optimization. *Advances in Neural Information Processing Systems*, 34:13670–13682, 2021.

[72] Yiming Ying, Longyin Wen, and Siwei Lyu. Stochastic online auc maximization. In *Advances in Neural Information Processing Systems*, pages 451–459, 2016.

[73] Zhuoning Yuan, Yan Yan, Milan Sonka, and Tianbao Yang. Large-scale robust deep auc maximization: A new surrogate loss and empirical studies on medical image classification. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 3040–3049, 2021.

[74] Bohang Zhang, Jikai Jin, Cong Fang, and Liwei Wang. Improved analysis of clipping algorithms for non-convex optimization. *Advances in Neural Information Processing Systems*, 33:15511–15521, 2020.

[75] Jingzhao Zhang, Tianxing He, Suvrit Sra, and Ali Jadbabaie. Why gradient clipping accelerates training: A theoretical justification for adaptivity. *International Conference on Learning Representations*, 2020.

A Technical Lemmas

In this section, we will introduce a few useful lemmas. The following technical lemma on recursive control is crucial for providing high probability guarantee of the lower-level variables y_t and $\hat{y}_t$ in Algorithm 2 at *anytime*. We follow a similar argument as in [20, Proposition 29] with a slight generalization.

Lemma A.1 (Recursive control on MGF)**.** *Consider scalar stochastic processes* (V_t), $(V'_{t,1})$, $(V'_{t,2})$, $(D_{t,1})$, $(D_{t,2})$ *and* (X_t) *on a probability space with filtration* $(\mathcal{H}_t)$*, which are linked by the inequality*

$$V_{t+1} \leq \alpha_t V_t + D_{t,1}\sqrt{V'_{t,1}} + D_{t,2}\sqrt{V'_{t,2}} + X_t + \kappa_t$$

for some deterministic constants $\alpha_t \in (-\infty, 1]$ *and* $\kappa_t \in \mathbb{R}$*. Suppose the following properties hold.*

- $V_t, V'_{t,1}$ *and* $V'_{t,2}$ *are non-negative and* $\mathcal{H}_t$*-measurable.*
- $D_{t,i}$ *is mean-zero sub-Gaussian conditioned on* $\mathcal{H}_t$ *with deterministic parameter* σ_i*, and* $V'_{t,i} \leq V_t$ *for* $i = 1, 2$*:*

$$\mathbb{E}[\exp(\lambda D_{t,i}) \mid \mathcal{H}_t] \leq \exp(\lambda^2\sigma_i^2/2) \quad \textit{for all} \quad \lambda \in \mathbb{R}.$$

- X_t *is non-negative and sub-exponential conditioned on* $\mathcal{H}_t$ *with deterministic parameter* ν_t*:*

$$\mathbb{E}[\exp(\lambda X_t) \mid \mathcal{H}_t] \leq \exp(\lambda\nu_t) \quad \textit{for all} \quad 0 \leq \lambda \leq 1/\nu_t.$$

Then the estimate

$$\mathbb{E}[\exp(\lambda V_{t+1})] \leq \exp(\lambda(\nu_t + \kappa_t))\mathbb{E}[\exp(\lambda(1+\alpha_t)V_t/2)]$$

holds for any λ *satisfying* $0 \leq \lambda \leq \min\left\{\frac{1-\alpha_t}{2(\sigma_1^2+\sigma_2^2)}, \frac{1}{2\nu_t}\right\}$.

Proof of Lemma A.1. For any index $t \geq 0$ and any scalar $\lambda \geq 0$, the law of total expectation implies

$$\begin{aligned}\mathbb{E}[\exp(\lambda V_{t+1})] &\leq \mathbb{E}\left[\exp(\lambda(\alpha_t V_t + D_{t,1}\sqrt{V'_{t,1}} + D_{t,2}\sqrt{V'_{t,2}} + X_t + \kappa_t))\right] \\ &= \exp(\lambda\kappa_t)\mathbb{E}\left[\exp(\lambda\alpha_t V_t)\mathbb{E}\left[\exp\left(\lambda\left(D_{t,1}\sqrt{V'_{t,1}} + D_{t,2}\sqrt{V'_{t,2}}\right)\right)\exp(\lambda X_t) \mid \mathcal{H}_t\right]\right].\end{aligned}$$

Hölder's inequality in turn yields

$$\begin{aligned}&\mathbb{E}\left[\exp(\lambda\alpha_t V_t)\mathbb{E}\left[\exp\left(\lambda\left(D_{t,1}\sqrt{V'_{t,1}} + D_{t,2}\sqrt{V'_{t,2}}\right)\right)\exp(\lambda X_t) \mid \mathcal{H}_t\right]\right] \\ &\quad\leq \sqrt{\mathbb{E}\left[\exp\left(2\lambda\left(D_{t,1}\sqrt{V'_{t,1}} + D_{t,2}\sqrt{V'_{t,2}}\right)\right) \mid \mathcal{H}_t\right] \cdot \mathbb{E}\left[\exp(2\lambda X_t) \mid \mathcal{H}_t\right]} \\ &\quad\leq \sqrt{\exp\left(2\lambda^2(\sigma_i^2 V'_{t,1} + \sigma_i^2 V'_{t,2})\right)\exp(2\lambda\nu_t)} \\ &\quad\leq \exp\left(\lambda^2(\sigma_1^2+\sigma_2^2)V_t\right)\exp(\lambda\nu_t)\end{aligned}$$

provided $0 \leq \lambda \leq 1/2\nu_t$, where we use $V'_{t,i} \leq V_t$ for $i = 1, 2$ in the last inequality. Therefore, under the condition that

$$0 \leq \lambda \leq \min\left\{\frac{1-\alpha_t}{2(\sigma_1^2+\sigma_2^2)}, \frac{1}{2\nu_t}\right\},$$

the following estimate hold for all $t \geq 0$:

$$\begin{aligned}\mathbb{E}[\exp(\lambda V_{t+1})] &\leq \exp(\lambda\kappa_t)\mathbb{E}\left[\exp(\lambda\alpha_t V_t)\exp\left(\lambda^2(\sigma_1^2+\sigma_2^2)V_t\right)\exp(\lambda\nu_t)\right] \\ &= \exp(\lambda(\nu_t+\kappa_t))\mathbb{E}\left[\exp\left(\lambda(\alpha_t + \lambda(\sigma_1^2+\sigma_2^2))V_t\right)\right] \\ &\leq \exp(\lambda(\nu_t+\kappa_t))\mathbb{E}[\exp(\lambda(1+\alpha_t)V_t/2)],\end{aligned}$$

where the last inequality follows by the given range of λ. Thus the proof is completed. □

Next, we introduce the following Young's inequality beyond Euclidean norm cases. This lemma serves as an important role when dealing with distributional drift for high probability SNAG analysis.

Lemma A.2 (Young's inequality)**.** *For any vectors $v_1, v_2 \in \mathbb{R}^d$, positive semidefinite (PSD) matrix $\mathbf{Q} \in \mathbb{R}^{d\times d}$, and scalar $c > 0$, it holds that* [4]

$$\|v_1 + v_2\|_{\mathbf{Q}}^2 \le (1 + c)\|v_1\|_{\mathbf{Q}}^2 + \left(1 + \frac{1}{c}\right)\|v_2\|_{\mathbf{Q}}^2.$$

Proof of Lemma A.2. By definition of $\|\cdot\|_{\mathbf{Q}}$, we have

$$\begin{aligned}\|v_1 + v_2\|_{\mathbf{Q}}^2 &= (v_1 + v_2)^\top \mathbf{Q}(v_1 + v_2)\\ &= \|v_1\|_{\mathbf{Q}}^2 + \|v_2\|_{\mathbf{Q}}^2 + 2v_1^\top \mathbf{Q}v_2.\end{aligned} \tag{6}$$

Since $\mathbf{Q} \in \mathbb{R}^{d\times d}$ is PSD, let $\mathbf{Q} = \mathbf{U}\mathbf{U}^\top$ be the Cholesky decomposition, then

$$\begin{aligned}2v_1^\top \mathbf{Q}v_2 &= 2v_1^\top \mathbf{U}\mathbf{U}^\top v_2 = 2(\mathbf{U}^\top v_1)^\top(\mathbf{U}^\top v_2)\\ &\le c\|\mathbf{U}^\top v_1\|^2 + \frac{1}{c}\|\mathbf{U}^\top v_2\|^2\\ &= c\|v_1\|_{\mathbf{Q}}^2 + \frac{1}{c}\|v_2\|_{\mathbf{Q}}^2,\end{aligned} \tag{7}$$

where we use Young's inequality and definition of $\|\cdot\|_{\mathbf{Q}}$ for the second and third lines, respectively. Combing (6) and (7) gives the result as claimed. □

B Auxiliary Lemmas for Bilevel Optimization

In this section, we provide important properties of the objective function Φ in bilevel optimization problems, as well as characterizations (such as variance and bias) for stochastic hypergradient estimator $\bar{\nabla} f(x, y; \bar{\xi})$ based on Neumann series. For readers' convenience, we only list the results here and defer the detailed proofs to Appendix F.

Lemma B.1 (Lipschitz property, [38, Lemma 8])**.** *Under Assumptions 3.1 and 3.2, $y^*(x)$ is $(l_{g,1}/\mu)$-Lipschitz continuous.*

Lemma B.2 ((L_0, L_1)-smoothness, [38, Lemma 9])**.** *Under Assumptions 3.1 and 3.2, for any x, x' we have*

$$\|\nabla\Phi(x) - \nabla\Phi(x')\| \le (L_0 + L_1\|\nabla\Phi(x')\|)\|x - x'\| \quad \textit{if} \quad \|x - x'\| \le \frac{1}{\sqrt{2(1 + l_{g,1}^2/\mu^2)(L_{x,1}^2 + L_{y,1}^2)}},$$

where (L_0, L_1)-smoothness constant L_0 and L_1 are defined as

$$L_0 = \sqrt{1 + \frac{l_{g,1}^2}{\mu^2}}\left(L_{x,0} + L_{x,1}\frac{l_{g,1}l_{f,0}}{\mu} + \frac{l_{g,1}}{\mu}(L_{y,0} + L_{y,1}l_{f,0}) + l_{f,0}\frac{l_{g,1}l_{g,2} + l_{g,2}\mu}{\mu^2}\right) \quad \textit{and} \quad L_1 = \sqrt{1 + \frac{l_{g,1}^2}{\mu^2}}L_{x,1}.$$

Lemma B.3 (Descent inequality, [38, Lemma 10])**.** *Suppose Assumptions 3.1 and 3.2 and 3.2 hold. Then for any x, x' we have*

$$\Phi(x) \le \Phi(x') + \langle\nabla\Phi(x'), x - x'\rangle + \frac{L_0 + L_1\|\nabla\Phi(x')\|}{2}\|x - x'\|^2 \quad \textit{if} \quad \|x - x'\| \le \frac{1}{\sqrt{2(1 + l_{g,1}^2/\mu^2)(L_{x,1}^2 + L_{y,1}^2)}}.$$

Lemma B.4 ([46, Lemma B.1])**.** *Under Assumptions 3.1 to 3.4, the bias of the stochastic hypergradient estimate of the upper-level objective satisfies*

$$\|\bar{\nabla} f(x, y) - \mathbb{E}_{\bar{\xi}}[\bar{\nabla} f(x, y; \bar{\xi})]\| \le \frac{l_{g,1}l_{f,0}}{\mu}\left(1 - \frac{\mu}{l_{g,1}}\right)^Q,$$

where Q is the number of samples chosen to approximate the Hessian inverse. Moreover, we have

$$\mathbb{E}_{\bar{\xi}}[\|\bar{\nabla} f(x, y; \bar{\xi}) - \mathbb{E}_{\bar{\xi}}[\bar{\nabla} f(x, y; \bar{\xi})]\|^2] \le \sigma_{f,1}^2 + \frac{3}{\mu^2}\left[(\sigma_{f,1}^2 + l_{f,0}^2)(\sigma_{g,2}^2 + 2l_{g,1}^2) + \sigma_{f,1}^2 l_{g,1}^2\right] := \bar{\sigma}^2.$$

[4] Here we define $\|v\|_{\mathbf{Q}} := \sqrt{v^\top \mathbf{Q}v}$ for any vector $v \in \mathbb{R}^d$ and PSD matrix $\mathbf{Q} \in \mathbb{R}^{d\times d}$.

Lemma B.5. *Under Assumptions 3.1 to 3.4, we have*

$$\|\bar{\nabla} f(x,y) - \nabla\Phi(x)\| \le (\bar{L} + L_{x,1}\|\nabla\Phi(x)\|)\|y - y^*(x)\|,$$

where constant $\bar{L}$ is defined as

$$\bar{L} := L_{x,0} + L_{x,1}\frac{l_{g,1}l_{f,0}}{\mu} + \frac{l_{g,1}}{\mu}(L_{y,0} + L_{y,1}l_{f,0}) + l_{f,0}\frac{\mu l_{g,2} + l_{g,1}l_{g,2}}{\mu^2} \le L_0.$$

Lemma B.6. *Under Assumptions 3.1 to 3.4, we have*

(i) For any fixed $y \in \mathbb{R}^{d_y}$ and any $x, x' \in \mathbb{R}^{d_x}$,

$$\mathbb{E}_{\bar{\xi}}\|\bar{\nabla} f(x,y;\bar{\xi}) - \bar{\nabla} f(x',y;\bar{\xi})\|^2 \le (\bar{L}_0^2 + \bar{L}_1^2\|\nabla\Phi(x)\|^2)\|x - x'\|^2.$$

(ii) For any fixed $x \in \mathbb{R}^{d_x}$ and any $y, y' \in \mathbb{R}^{d_y}$,

$$\mathbb{E}_{\bar{\xi}}\|\bar{\nabla} f(x,y;\bar{\xi}) - \bar{\nabla} f(x,y';\bar{\xi})\|^2 \le (\bar{L}_0^2 + \bar{L}_1^2\|\nabla\Phi(x)\|^2)\|y - y'\|^2.$$

In the above expressions, we define $\bar{L}_0$ and $\bar{L}_1$ as

$$\bar{L}_0 = \Bigg\{4\left(L_{x,0} + L_{x,1}\left(\frac{l_{g,1}l_{f,0}}{\mu} + \left(L_{x,0} + \frac{L_{x,1}l_{g,1}l_{f,0}}{\mu}\right)\|y - y^*(x)\|\right)\right)^2 + \frac{6Q}{2\mu l_{g,1} - \mu^2}\left(l_{g,1}^2(L_{y,0} + L_{y,1}l_{f,0})^2 + l_{f,0}^2 l_{g,2}^2 + \frac{l_{f,0}^2 l_{g,1}^2 l_{g,2}^2 Q^2}{(l_{g,1} - \mu)^2}\right)\Bigg\}^{1/2},$$

$$\bar{L}_1 = 2L_{x,1}(1 + L_{x,1}\|y - y^*(x)\|).$$

Note that in Lemma B.6, constant $\bar{L}_0$ depends on the value of $\|y - y^*(x)\|$. When we consider this term in Algorithm 2, it turns into $\|y_t - y_t^*\|$ or $\|\hat{y}_t - y_t^*\|$, which are both as small as $O(\epsilon)$ (and thus bounded) with high probability by Lemmas 4.5 to 4.7. In other words, we can treat this term as another constant for our algorithm and analysis.

C Proofs of Results in Section 4.3.1

For convenience, we will restate a few concepts included in Section 4.3.1 here. We consider the sequences of stochastic optimization problems

$$\min_{w \in \mathbb{R}^d} \phi_t(w) \tag{8}$$

indexed by time $t \in \mathbb{N}$. We denote the minimizer and the minimal value of ϕ_t as w_t^* and ϕ_t^*, and we define the *minimizer drift* at time t to be $\Delta_t := \|w_t^* - w_{t+1}^*\|$. With a slight abuse of notation, we consider the SNAG algorithm applied to the sequence $\{\phi_t\}_{t=1}^T$, where T is the total number of iterations:

$$\begin{aligned} z_t &= w_t + \gamma(w_t - w_{t-1}) \\ w_{t+1} &= w_t + \gamma(w_t - w_{t-1}) - \alpha g_t, \end{aligned} \tag{9}$$

where $g_t = \nabla\phi_t(z_t;\xi_t)$ is the stochastic gradient evaluated at z_t with random sample ξ_t. Define $\varepsilon_t = g_t - \nabla\phi_t(z_t)$ as the stochastic gradient noise at t-th iteration. Define $\mathcal{H}_t = \sigma(\xi_1, \ldots, \xi_{t-1})$ as the filtration, which is the σ-algebra generated by all random variables until t-th iteration. We will make the following standard assumption, as illustrated below [5].

Assumption C.1. *The sequences of time-varying functions satisfy that, each function $\phi_t : \mathbb{R}^d \to \mathbb{R}$ is μ-strongly convex and L-smooth for some constants $\mu, L > 0$.*

Assumption C.2 (Sub-Gaussian drift and noise)**.** *There exists constants $\Delta, \sigma > 0$ such that the following holds for all $t \ge 0$:*

*(i) (**Drift**) The drift Δ_t^2 is sub-exponential conditioned on $\mathcal{H}_t$ with parameter Δ^2:*

$$\mathbb{E}\left[\exp(\lambda\Delta_t^2) \mid \mathcal{H}_t\right] \le \exp(\lambda\Delta^2) \quad \textit{for all} \quad 0 \le \lambda \le \Delta^{-2}.$$

[5] Note that Assumptions C.1 and C.2 are more concrete than that in Section 4.3.1.

(ii) ***(Noise)*** *The noise ε_t is norm sub-Gaussian conditioned on $\mathcal{H}_t$ with parameter $\sigma/2$:*

$$\Pr\{\|\varepsilon_t\| \geq \varrho \mid \mathcal{H}_t\} \leq 2\exp(-2\varrho^2/\sigma^2) \quad \textit{for all} \quad \varrho > 0.$$

The following lemma characterize the one-step improvement for stochastic Nesterov accelerated gradient method. Although part of our analysis is similar to [13, 5], our final goal is quite different: we aim to derive a careful formulation (see (13)) such that we can apply Lemma A.1 to recursively control the moment generating function of V_t with distributional drift, thus leading to a high probability bound for V_t at *anytime* (see Lemma C.5), while [13, 5] only show the convergence in expectation without distributional drift.

Lemma C.3 (Distance recursion, with drift)**.** *Suppose that Assumptions C.1 and C.2 hold. Let $\{w_t\}$ be the iterates produced by update rule* (9) *with constant learning rate $\alpha \leq 1/2L$ and set constants $\gamma, \rho > 0$, and matrix $\mathbf{P} \in \mathbb{R}^{2d\times 2d}$ as*

$$\gamma = \frac{1-\sqrt{\mu\alpha}}{1+\sqrt{\mu\alpha}}, \quad \rho^2 = 1-\sqrt{\mu\alpha}, \quad \mathbf{P} = \frac{1}{2\alpha}\begin{bmatrix} 1 & \sqrt{\mu\alpha}-1 \\ \sqrt{\mu\alpha}-1 & (1-\sqrt{\mu\alpha})^2 \end{bmatrix} \otimes \mathbf{I}_d. \tag{10}$$

Define $\theta_t = [(w_t - w_t^*)^\top, (w_{t-1} - w_t^*)^\top]^\top \in \mathbb{R}^{2d}$, also define the potential function and $u_{t,1}, u_{t,2}$ as

$$V_t = \theta_t^\top \mathbf{P}\theta_t + \phi_t(w_t) - \phi_t(w_t^*), \qquad u_{t,1} = \frac{w_t - w_t^*}{\|w_t - w_t^*\|}, \qquad u_{t,2} = \frac{z_t - w_t}{\|z_t - w_t\|}. \tag{11}$$

Then for all $t \geq 0$, it holds that

$$\begin{aligned} &\begin{bmatrix} w_{t+1} - w_t^* \\ w_t - w_t^* \end{bmatrix}^\top \mathbf{P} \begin{bmatrix} w_{t+1} - w_t^* \\ w_t - w_t^* \end{bmatrix} + \phi_t(w_{t+1}) - \phi_t(w_t^*) \\ &\qquad\qquad \leq \rho^2 V_t - \alpha(1-L\alpha)\langle \nabla\phi_t(z_t), \varepsilon_t\rangle + \frac{L\alpha^2}{2}\|\varepsilon_t\|^2. \end{aligned} \tag{12}$$

Specifically, if $\phi_t(w) \coloneqq \frac{\mu}{2}\|w - w_t^*\|^2$, then we have

$$\begin{aligned} V_{t+1} \leq \left(1 - \frac{\sqrt{\mu\alpha}}{2}\right) V_t + \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) \Bigg[&-\sqrt{2\mu}\alpha(1-L\alpha)\langle u_{t,1}, \varepsilon_t\rangle \sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \\ &- \frac{2\mu\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\langle u_{t,2}, \varepsilon_t\rangle \frac{1+\sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t - w_t\| + \frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2 \Bigg] + \frac{20\mu\Delta_t^2}{\sqrt{\mu\alpha}}. \end{aligned} \tag{13}$$

Proof of Lemma C.3. We first apply Lemma A.2 with

$$v_1 + v_2 = \theta_{t+1} = \begin{bmatrix} w_{t+1} - w_{t+1}^* \\ w_t - w_{t+1}^* \end{bmatrix}, \quad v_1 = \begin{bmatrix} w_{t+1} - w_t^* \\ w_t - w_t^* \end{bmatrix}, \quad v_2 = \begin{bmatrix} w_t^* - w_{t+1}^* \\ w_t^* - w_{t+1}^* \end{bmatrix}, \quad \mathbf{Q} = \mathbf{P}$$

to obtain

$$\begin{aligned} &V_{t+1} = \theta_{t+1}^\top \mathbf{P}\theta_{t+1} + \phi_{t+1}(w_{t+1}) - \phi_{t+1}(w_{t+1}^*) \\ &\leq \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) \begin{bmatrix} w_{t+1} - w_t^* \\ w_t - w_t^* \end{bmatrix}^\top \mathbf{P} \begin{bmatrix} w_{t+1} - w_t^* \\ w_t - w_t^* \end{bmatrix} + \left(1 + \frac{4}{\sqrt{\mu\alpha}}\right) \begin{bmatrix} w_t^* - w_{t+1}^* \\ w_t^* - w_{t+1}^* \end{bmatrix}^\top \mathbf{P} \begin{bmatrix} w_t^* - w_{t+1}^* \\ w_t^* - w_{t+1}^* \end{bmatrix} + \phi_{t+1}(w_{t+1}) - \phi_{t+1}(w_{t+1}^*) \\ &= \underbrace{\left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) \left\{ \begin{bmatrix} w_{t+1} - w_t^* \\ w_t - w_t^* \end{bmatrix}^\top \mathbf{P} \begin{bmatrix} w_{t+1} - w_t^* \\ w_t - w_t^* \end{bmatrix} + \phi_t(w_{t+1}) - \phi_t(w_t^*) \right\}}_{(A)} \\ &\quad + \underbrace{\phi_{t+1}(w_{t+1}) - \phi_{t+1}(w_{t+1}^*) - \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)(\phi_t(w_{t+1}) - \phi_t(w_t^*))}_{(B)} + \underbrace{\left(1 + \frac{4}{\sqrt{\mu\alpha}}\right) \begin{bmatrix} w_t^* - w_{t+1}^* \\ w_t^* - w_{t+1}^* \end{bmatrix}^\top \mathbf{P} \begin{bmatrix} w_t^* - w_{t+1}^* \\ w_t^* - w_{t+1}^* \end{bmatrix}}_{(C)}. \end{aligned}$$

Now we bound terms (A), (B) and (C) individually.

Bounding (A)**.** Let us define vector $\omega_t \in \mathbb{R}^d$ and matrices $\mathbf{A} \in \mathbb{R}^{2d\times 2d}, \mathbf{B} \in \mathbb{R}^{2d\times d}$ as

$$\omega_t = \nabla\phi_t(z_t), \quad \mathbf{A} = \begin{bmatrix} 1+\gamma & -\gamma \\ 1 & 0 \end{bmatrix} \otimes \mathbf{I}_d, \quad \mathbf{B} = \begin{bmatrix} -\alpha \\ 0 \end{bmatrix} \otimes \mathbf{I}_d.$$

By (9) we have

$$[(w_{t+1} - w_t^*)^\top, (w_t - w_t^*)^\top]^\top = \mathbf{A}\theta_t + \mathbf{B}(\omega_t + \varepsilon_t) \tag{14}$$

Since ϕ_t is μ-strongly convex, then

$$\phi_t(w_t) - \phi_t(z_t) \geq \langle \nabla\phi_t(z_t), w_t - z_t\rangle + \frac{\mu}{2}\|w_t - z_t\|^2. \tag{15}$$

By L-smoothness of ϕ_t and the fact that $w_{t+1} = z_t - \alpha g_t$, we have

$$\begin{aligned}
\phi_t(z_t) - \phi_t(w_{t+1}) &\geq \langle \nabla\phi_t(z_t), z_t - w_{t+1}\rangle - \frac{L}{2}\|w_{t+1} - z_t\|^2 \\
&= \alpha\langle \nabla\phi_t(z_t), g_t\rangle - \frac{L\alpha^2}{2}\|g_t\|^2 \\
&= \alpha\|\nabla\phi_t(z_t)\|^2 + \alpha\langle \nabla\phi_t(z_t), \varepsilon_t\rangle - \frac{L\alpha^2}{2}(\|\nabla\phi_t(z_t)\|^2 + 2\langle \nabla\phi_t(z_t), \varepsilon_t\rangle + \|\varepsilon_t\|^2) \\
&= \frac{\alpha}{2}(2 - L\alpha)\|\nabla\phi_t(z_t)\|^2 - \frac{L\alpha^2}{2}\|\varepsilon_t\|^2 + \alpha(1 - L\alpha)\langle \nabla\phi_t(z_t), \varepsilon_t\rangle,
\end{aligned} \tag{16}$$

where we use $g_t = \nabla\phi_t(z_t) + \varepsilon_t$ in the second equality. Noting that by (9) we have

$$w_t - z_t = -\gamma(w_t - w_t^*) + \gamma(w_{t-1} - w_t^*),$$

and combining (15) and (16) we obtain

$$\begin{aligned}
\phi_t(w_t) - \phi_t(w_{t+1}) &\geq \langle \nabla\phi_t(z_t), w_t - z_t\rangle + \frac{\mu}{2}\|w_t - z_t\|^2 \\
&\quad + \frac{\alpha}{2}(2 - L\alpha)\|\nabla\phi_t(z_t)\|^2 - \frac{L\alpha^2}{2}\|\varepsilon_t\|^2 + \alpha(1 - L\alpha)\langle \nabla\phi_t(z_t), \varepsilon_t\rangle \\
&= \begin{bmatrix} \theta_t \\ \omega_t \end{bmatrix}^\top \mathbf{X}_1 \begin{bmatrix} \theta_t \\ \omega_t \end{bmatrix} - \frac{L\alpha^2}{2}\|\varepsilon_t\|^2 + \alpha(1 - L\alpha)\langle \nabla\phi_t(z_t), \varepsilon_t\rangle,
\end{aligned} \tag{17}$$

where matrix $\mathbf{X}_1 \in \mathbb{R}^{3d\times 3d}$ is defined as

$$\mathbf{X}_1 = \frac{1}{2}\begin{bmatrix} \mu\gamma^2 & -\mu\gamma^2 & -\gamma \\ -\mu\gamma^2 & \mu\gamma^2 & \gamma \\ -\gamma & \gamma & \alpha(2 - L\alpha) \end{bmatrix} \otimes \mathbf{I}_d.$$

Then applying the strong convexity of ϕ_t again gives

$$\phi_t(w_t^*) - \phi_t(z_t) \geq \langle \nabla\phi_t(z_t), w_t^* - z_t\rangle + \frac{\mu}{2}\|w_t^* - z_t\|^2. \tag{18}$$

Noting that

$$\begin{aligned}
w_t^* - z_t &= (w_t^* - w_t) - \gamma(w_t - w_t^*) + \gamma(w_{t-1} - w_t^*) \\
&= -(1+\gamma)(w_t - w_t^*) + \gamma(w_{t-1} - w_t^*),
\end{aligned}$$

and combining (16) and (18) we obtain

$$\begin{aligned}
\phi_t(w_t^*) - \phi_t(w_{t+1}) &\geq \langle \nabla\phi_t(z_t), w_t^* - z_t\rangle + \frac{\mu}{2}\|w_t^* - z_t\|^2 \\
&\quad + \frac{\alpha}{2}(2 - L\alpha)\|\nabla\phi_t(z_t)\|^2 - \frac{L\alpha^2}{2}\|\varepsilon_t\|^2 + \alpha(1 - L\alpha)\langle \nabla\phi_t(z_t), \varepsilon_t\rangle \\
&= \begin{bmatrix} \theta_t \\ \omega_t \end{bmatrix}^\top \mathbf{X}_2 \begin{bmatrix} \theta_t \\ \omega_t \end{bmatrix} - \frac{L\alpha^2}{2}\|\varepsilon_t\|^2 + \alpha(1 - L\alpha)\langle \nabla\phi_t(z_t), \varepsilon_t\rangle,
\end{aligned} \tag{19}$$

where matrix $\mathbf{X}_2 \in \mathbb{R}^{3d\times 3d}$ is defined as

$$\mathbf{X}_2 = \frac{1}{2}\begin{bmatrix} \mu(1+\gamma)^2 & -\mu\gamma(1+\gamma) & -(1+\gamma) \\ -\mu\gamma(1+\gamma) & \mu\gamma^2 & \gamma \\ -(1+\gamma) & \gamma & \alpha(2 - L\alpha) \end{bmatrix} \otimes \mathbf{I}_d.$$

Next, we multiply (17) by ρ^2 and (19) by $1-\rho^2$, then sum them up to get

$$\begin{aligned}&\rho^2(\phi_t(w_t)-\phi_t(w_t^*))-(\phi_t(w_{t+1})-\phi_t(w_t^*))\\&\qquad\geq\begin{bmatrix}\theta_t\\\omega_t\end{bmatrix}^\top(\rho^2\mathbf{X}_1+(1-\rho^2)\mathbf{X}_2)\begin{bmatrix}\theta_t\\\omega_t\end{bmatrix}-\frac{L\alpha^2}{2}\|\varepsilon_t\|^2+\alpha(1-L\alpha)\langle\nabla\phi_t(z_t),\varepsilon_t\rangle.\end{aligned}\tag{20}$$

By [42, Section 3.1] (see also [5, Corollary 4.9], [4, Theorem 2.3]), we have the following fact:

$$\begin{bmatrix}\mathbf{A}^\top\mathbf{P}\mathbf{A}-\rho^2\mathbf{P} & \mathbf{A}^\top\mathbf{P}\mathbf{B}\\ \mathbf{B}^\top\mathbf{P}\mathbf{A} & \mathbf{B}^\top\mathbf{P}\mathbf{B}\end{bmatrix}-(\rho^2\mathbf{X}_1+(1-\rho^2)\mathbf{X}_2)\preceq 0,\tag{21}$$

which, combined with (20) yields

$$\begin{aligned}&\begin{bmatrix}w_{t+1}-w_t^*\\w_t-w_t^*\end{bmatrix}^\top\mathbf{P}\begin{bmatrix}w_{t+1}-w_t^*\\w_t-w_t^*\end{bmatrix}-\rho^2\theta_t^\top\mathbf{P}\theta_t\\&=\begin{bmatrix}\theta_t\\\omega_t\end{bmatrix}^\top\begin{bmatrix}\mathbf{A}^\top\mathbf{P}\mathbf{A}-\rho^2\mathbf{P} & \mathbf{A}^\top\mathbf{P}\mathbf{B}\\ \mathbf{B}^\top\mathbf{P}\mathbf{A} & \mathbf{B}^\top\mathbf{P}\mathbf{B}\end{bmatrix}\begin{bmatrix}\theta_t\\\omega_t\end{bmatrix}+\varepsilon_t^\top\mathbf{B}^\top\mathbf{P}\mathbf{B}\varepsilon_t\\&\leq\begin{bmatrix}\theta_t\\\omega_t\end{bmatrix}^\top(\rho^2\mathbf{X}_1+(1-\rho^2)\mathbf{X}_2)\begin{bmatrix}\theta_t\\\omega_t\end{bmatrix}+\frac{\alpha}{2}\|\varepsilon_t\|^2\\&\leq-(\phi_t(w_{t+1})-\phi_t(w_t^*))+\rho^2(\phi_t(w_t)-\phi_t(w_t^*))-\alpha(1-L\alpha)\langle\nabla\phi_t(z_t),\varepsilon_t\rangle+\frac{\alpha+L\alpha^2}{2}\|\varepsilon_t\|^2,\end{aligned}$$

where the first inequality uses (14) and (21), along with the fact that $\mathbf{B}^\top\mathbf{P}\mathbf{B}=(\alpha/2)\otimes\mathbf{I}_d$ and hence $\lambda_{\max}(\mathbf{B}^\top\mathbf{P}\mathbf{B})=\alpha/2$; and the last inequality follows by (20). Rearrange the above inequality and by definition of the potential function V_t, we obtain

$$\begin{aligned}&\begin{bmatrix}w_{t+1}-w_t^*\\w_t-w_t^*\end{bmatrix}^\top\mathbf{P}\begin{bmatrix}w_{t+1}-w_t^*\\w_t-w_t^*\end{bmatrix}+\phi_t(w_{t+1})-\phi_t(w_t^*)\\&\qquad\leq\rho^2V_t-\alpha(1-L\alpha)\langle\nabla\phi_t(z_t),\varepsilon_t\rangle+\frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2.\end{aligned}\tag{22}$$

Now recall that in (8) our objective function has the form of $\phi_t(w)=\frac{\mu}{2}\|w-w_t^*\|^2$, hence $\nabla\phi_t(z_t)=\mu(z_t-w_t^*)$. Plugging this into the above inequality gives

$$\begin{aligned}&\begin{bmatrix}w_{t+1}-w_t^*\\w_t-w_t^*\end{bmatrix}^\top\mathbf{P}\begin{bmatrix}w_{t+1}-w_t^*\\w_t-w_t^*\end{bmatrix}+\phi_t(w_{t+1})-\phi_t(w_t^*)\\&\quad\leq\rho^2V_t-\mu\alpha(1-L\alpha)\langle z_t-w_t^*,\varepsilon_t\rangle+\frac{\alpha+L\alpha^2}{2}\|\varepsilon_t\|^2\\&\quad=\rho^2V_t-\mu\alpha(1-L\alpha)\langle w_t-w_t^*,\varepsilon_t\rangle-\mu\alpha(1-L\alpha)\langle z_t-w_t,\varepsilon_t\rangle+\frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2\\&\quad=\rho^2V_t-\sqrt{2\mu}\alpha(1-L\alpha)\langle u_{t,1},\varepsilon_t\rangle\sqrt{\frac{\mu}{2}}\|w_t-w_t^*\|\\&\qquad-\frac{2\mu\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\langle u_{t,2},\varepsilon_t\rangle\frac{1+\sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t-w_t\|+\frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2,\end{aligned}\tag{23}$$

where $u_{t,1}$ and $u_{t,2}$ are defined as

$$u_{t,1}=\frac{w_t-w_t^*}{\|w_t-w_t^*\|},\qquad u_{t,2}=\frac{z_t-w_t}{\|z_t-w_t\|}.$$

Therefore, we conclude that

$$\begin{aligned}(A)&\leq\left(1+\frac{\sqrt{\mu\alpha}}{4}\right)\Bigg[\rho^2V_t-\sqrt{2\mu}\alpha(1-L\alpha)\langle u_{t,1},\varepsilon_t\rangle\sqrt{\frac{\mu}{2}}\|w_t-w_t^*\|\\&\qquad-\frac{2\mu\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\langle u_{t,2},\varepsilon_t\rangle\frac{1+\sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t-w_t\|+\frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2\Bigg]\\&\leq\left(1-\frac{3\sqrt{\mu\alpha}}{4}\right)V_t+\Bigg[-\sqrt{2\mu}\alpha(1-L\alpha)\langle u_{t,1},\varepsilon_t\rangle\sqrt{\frac{\mu}{2}}\|w_t-w_t^*\|\\&\qquad-\frac{2\mu\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\langle u_{t,2},\varepsilon_t\rangle\frac{1+\sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t-w_t\|+\frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2\Bigg],\end{aligned}\tag{24}$$

where the last inequality follows from the definition of ρ and simple calculation

$$\left(1+\frac{\sqrt{\mu\alpha}}{4}\right)\rho^2 = \left(1+\frac{\sqrt{\mu\alpha}}{4}\right)(1-\sqrt{\mu\alpha}) \le 1-\frac{3\sqrt{\mu\alpha}}{4}.$$

Bounding (B)**.** Recall that under distributional drift, the objective function in (8) has the form of $\phi_t(w) = \frac{\mu}{2}\|w - w_t^*\|^2$, then we have

$$\begin{aligned}
(B) &= \phi_{t+1}(w_{t+1}) - \phi_{t+1}(w_{t+1}^*) - \left(1+\frac{\sqrt{\mu\alpha}}{4}\right)(\phi_t(w_{t+1}) - \phi_t(w_t^*)) \\
&\le \left(1+\frac{\sqrt{\mu\alpha}}{4}\right)(\phi_{t+1}(w_{t+1}) - \phi_{t+1}(w_{t+1}^*) - \phi_t(w_{t+1}) + \phi_t(w_t^*)) \\
&= \frac{\mu}{2}\left(1+\frac{\sqrt{\mu\alpha}}{4}\right)(\|w_{t+1} - w_{t+1}^*\|^2 - \|w_{t+1} - w_t^*\|^2) \\
&\le \frac{\mu}{2}\left(1+\frac{\sqrt{\mu\alpha}}{4}\right)\|w_t^* - w_{t+1}^*\|\|w_{t+1} - w_t^* + w_{t+1} - w_{t+1}^*\| \\
&\le \frac{\mu}{2}\left(1+\frac{\sqrt{\mu\alpha}}{4}\right)\Delta_t(2\|w_{t+1} - w_{t+1}^*\| + \|w_{t+1}^* - w_t^*\|)
\end{aligned}$$

Since ϕ_{t+1} is μ-strongly convex and matrix $\mathbf{P}$ is PSD, then

$$\begin{aligned}
V_{t+1} &= \theta_{t+1}^\top \mathbf{P}\theta_{t+1} + \phi_{t+1}(w_{t+1}) - \phi_t(w_{t+1}^*) \ge \phi_{t+1}(w_{t+1}) - \phi_t(w_{t+1}^*) \\
&\ge \frac{\mu}{2}\|w_{t+1} - w_{t+1}^*\|^2 \qquad \Longrightarrow \qquad \|w_{t+1} - w_{t+1}^*\| \le \sqrt{\frac{2}{\mu}}\sqrt{V_{t+1}}.
\end{aligned}$$

Plugging the above fact back into the upper bound for (B) gives

$$\begin{aligned}
(B) &\le \frac{\mu}{2}\left(1+\frac{\sqrt{\mu\alpha}}{4}\right)\Delta_t\left(2\sqrt{\frac{2}{\mu}}\sqrt{V_{t+1}} + \Delta_t\right) \\
&= \sqrt{2\mu}\Delta_t\left(1+\frac{\sqrt{\mu\alpha}}{4}\right)\sqrt{V_{t+1}} + \frac{\mu}{2}\left(1+\frac{\sqrt{\mu\alpha}}{4}\right)\Delta_t^2.
\end{aligned} \tag{25}$$

Bounding (C)**.** For this part, we handle the distributional drift. By definition of $\mathbf{P}$ in (10), we have

$$\begin{aligned}
(C) &= \left(1+\frac{4}{\sqrt{\mu\alpha}}\right)\begin{bmatrix} w_t^* - w_{t+1}^* \\ w_t^* - w_{t+1}^* \end{bmatrix}^\top \frac{1}{2\alpha}\begin{bmatrix} \mathbf{I}_d & (\sqrt{\mu\alpha}-1)\mathbf{I}_d \\ (\sqrt{\mu\alpha}-1)\mathbf{I}_d & (1-\sqrt{\mu\alpha})^2\mathbf{I}_d \end{bmatrix}\begin{bmatrix} w_t^* - w_{t+1}^* \\ w_t^* - w_{t+1}^* \end{bmatrix} \\
&= \frac{\mu}{2}\left(1+\frac{4}{\sqrt{\mu\alpha}}\right)\Delta_t^2,
\end{aligned} \tag{26}$$

where in the last equality we use the basic algebra of block matrix multiplication and the definition of $\Delta_t = \|w_t^* - w_{t+1}^*\|$.

Final Bound for V_{t+1}**.** Now we are ready to derive the upper bound for V_{t+1}. Combining (24), (25) and (26) together yields

$$\begin{aligned}
V_{t+1} &\le (A) + (B) + (C) \\
&\le \left(1-\frac{3\sqrt{\mu\alpha}}{4}\right)V_t + \Bigg[-\sqrt{2\mu}\alpha(1-L\alpha)\langle u_{t,1}, \varepsilon_t\rangle\sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \\
&\qquad -\frac{2\mu\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\langle u_{t,2}, \varepsilon_t\rangle\frac{1+\sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t - w_t\| + \frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2\Bigg] \\
&\quad + \sqrt{2\mu}\Delta_t\left(1+\frac{\sqrt{\mu\alpha}}{4}\right)\sqrt{V_{t+1}} + \mu\left(1+\frac{\sqrt{\mu\alpha}}{8}+\frac{2}{\sqrt{\mu\alpha}}\right)\Delta_t^2.
\end{aligned} \tag{27}$$

For simplicity, we define D as the following

$$\begin{aligned}
D = &\left(1-\frac{3\sqrt{\mu\alpha}}{4}\right)V_t + \Bigg[-\sqrt{2\mu}\alpha(1-L\alpha)\langle u_{t,1}, \varepsilon_t\rangle\sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \\
&-\frac{2\mu\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\langle u_{t,2}, \varepsilon_t\rangle\frac{1+\sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t - w_t\| + \frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2\Bigg] + \mu\left(1+\frac{\sqrt{\mu\alpha}}{8}+\frac{2}{\sqrt{\mu\alpha}}\right)\Delta_t^2.
\end{aligned}$$

Hence (27) turns into

$$V_{t+1} - \sqrt{2\mu}\Delta_t \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) \sqrt{V_{t+1}} - D \leq 0.$$

Solving the above inequality we get

$$\begin{aligned}\sqrt{V_{t+1}} &\leq \frac{1}{2}\left[\sqrt{2\mu}\Delta_t \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) + \sqrt{\left(\sqrt{2\mu}\Delta_t \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\right)^2 + 4D}\right] \\ &\leq \sqrt{2\mu}\Delta_t \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) + \sqrt{D}\end{aligned}$$

Then an application of Young's inequality reveals

$$\begin{aligned}V_{t+1} &\leq \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) D + \left(1 + \frac{4}{\sqrt{\mu\alpha}}\right) \left(\sqrt{2\mu}\Delta_t \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\right)^2 \\ &= \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) \Bigg\{ \left(1 - \frac{3\sqrt{\mu\alpha}}{4}\right) V_t + \Bigg[-\sqrt{2\mu}\alpha(1 - L\alpha)\langle u_{t,1}, \varepsilon_t\rangle \sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \\ &\quad - \frac{2\mu\sqrt{2\alpha}}{1 + \sqrt{\mu\alpha}}\alpha(1 - L\alpha)\langle u_{t,2}, \varepsilon_t\rangle \frac{1 + \sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t - w_t\| + \frac{\alpha(1 + L\alpha)}{2}\|\varepsilon_t\|^2 \Bigg] + \mu\left(1 + \frac{\sqrt{\mu\alpha}}{8} + \frac{2}{\sqrt{\mu\alpha}}\right)\Delta_t^2 \Bigg\} \\ &\quad + \left(1 + \frac{4}{\sqrt{\mu\alpha}}\right) 2\mu\Delta_t^2 \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)^2 \\ &\leq \left(1 - \frac{\sqrt{\mu\alpha}}{2}\right) V_t + \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) \Bigg[-\sqrt{2\mu}\alpha(1 - L\alpha)\langle u_{t,1}, \varepsilon_t\rangle \sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \\ &\quad - \frac{2\mu\sqrt{2\alpha}}{1 + \sqrt{\mu\alpha}}\alpha(1 - L\alpha)\langle u_{t,2}, \varepsilon_t\rangle \frac{1 + \sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t - w_t\| + \frac{\alpha(1 + L\alpha)}{2}\|\varepsilon_t\|^2 \Bigg] \\ &\quad + \mu\left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\left(1 + \frac{\sqrt{\mu\alpha}}{8} + \frac{2}{\sqrt{\mu\alpha}}\right)\Delta_t^2 + \left(1 + \frac{4}{\sqrt{\mu\alpha}}\right) 2\mu\Delta_t^2 \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)^2,\end{aligned}$$

where we plug in the definition of D for the first equality. Since the learning rate $\alpha \leq 1/L$ and thus $\mu\alpha \leq 1$, then we have

$$\left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\left(1 + \frac{\sqrt{\mu\alpha}}{8} + \frac{2}{\sqrt{\mu\alpha}}\right) \leq \frac{125}{32\sqrt{\mu\alpha}}, \qquad 2\left(1 + \frac{4}{\sqrt{\mu\alpha}}\right)\left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)^2 \leq \frac{125}{8\sqrt{\mu\alpha}}.$$

Therefore, we finally conclude that

$$\begin{aligned}V_{t+1} &\leq \left(1 - \frac{\sqrt{\mu\alpha}}{2}\right) V_t + \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right) \Bigg[-\sqrt{2\mu}\alpha(1 - L\alpha)\langle u_{t,1}, \varepsilon_t\rangle \sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \\ &\quad - \frac{2\mu\sqrt{2\alpha}}{1 + \sqrt{\mu\alpha}}\alpha(1 - L\alpha)\langle u_{t,2}, \varepsilon_t\rangle \frac{1 + \sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t - w_t\| + \frac{\alpha(1 + L\alpha)}{2}\|\varepsilon_t\|^2 \Bigg] + \frac{20\mu\Delta_t^2}{\sqrt{\mu\alpha}},\end{aligned}$$

which is as claimed in (13). □

When there is no drift, the following lemma holds for any general strongly convex functions ϕ in $\mathbb{R}^d$.

Lemma C.4 (Distance recursion, without drift)**.** *Under the same settings as in Lemma C.3 with $\phi_t(w) \equiv \phi(w)$, and $w_t^* \equiv w^*$, where $\phi(w)$ can be any general strongly functions in $\mathbb{R}^d$. We redefine $u_{t,1}, u_{t,2}$ as*

$$u_{t,1} = \frac{\nabla\phi(w_t) - \nabla\phi(w^*)}{\|\nabla\phi(w_t) - \nabla\phi(w^*)\|}, \qquad u_{t,2} = \frac{\nabla\phi(z_t) - \nabla\phi(w_t)}{\|\nabla\phi(z_t) - \nabla\phi(w_t)\|}. \tag{28}$$

Then for all $t \geq 0$, it holds that

$$\begin{aligned}V_{t+1} &\leq (1 - \sqrt{\mu\alpha})V_t - \sqrt{\frac{2}{\mu}}L\alpha(1 - L\alpha)\langle u_{t,1}, \varepsilon_t\rangle \frac{1}{L}\sqrt{\frac{\mu}{2}}\|\nabla\phi_t(w_t) - \nabla\phi_t(w^*)\| \\ &\quad - \frac{2L\sqrt{2\alpha}}{1 + \sqrt{\mu\alpha}}\alpha(1 - L\alpha)\langle u_{t,2}, \varepsilon_t\rangle \frac{1 + \sqrt{\mu\alpha}}{2L\sqrt{2\alpha}}\|\nabla\phi_t(z_t) - \nabla\phi_t(w_t)\| + \frac{\alpha(1 + L\alpha)}{2}\|\varepsilon_t\|^2.\end{aligned} \tag{29}$$

Proof of Lemma C.4. By (12) in Lemma C.3 with $\phi_t(w) \equiv \phi(w)$ and $w_t^* \equiv w^*$, we have

$$\begin{aligned}
V_{t+1} &\le \rho^2 V_t - \alpha(1-L\alpha)\langle \nabla\phi_t(z_t), \varepsilon_t\rangle + \frac{L\alpha^2}{2}\|\varepsilon_t\|^2 \\
&= \rho^2 V_t - \alpha(1-L\alpha)\langle \nabla\phi_t(w_t) - \nabla\phi_t(w^*), \varepsilon_t\rangle - \alpha(1-L\alpha)\langle \nabla\phi_t(z_t) - \nabla\phi_t(w_t), \varepsilon_t\rangle + \frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2 \\
&= (1-\sqrt{\mu\alpha})V_t - \sqrt{\frac{2}{\mu}}L\alpha(1-L\alpha)\langle u_{t,1}, \varepsilon_t\rangle \frac{1}{L}\sqrt{\frac{\mu}{2}}\|\nabla\phi_t(w_t) - \nabla\phi_t(w^*)\| \\
&\quad - \frac{2L\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\langle u_{t,2}, \varepsilon_t\rangle \frac{1+\sqrt{\mu\alpha}}{2L\sqrt{2\alpha}}\|\nabla\phi_t(z_t) - \nabla\phi_t(w_t)\| + \frac{\alpha(1+L\alpha)}{2}\|\varepsilon_t\|^2.
\end{aligned}$$

Hence the proof is completed. □

The following result shows the first part of Lemma 4.3. To the best of our knowledge, this is the first high probability guarantee with improved rate for SNAG under distributional drift.

Lemma C.5 (High-probability distance tracking, with drift)**.** *Under the same setting as in Lemma C.3 with $\alpha \le 1/25L$, for any given $\delta \in (0,1)$ and all $t \in [T]$, the following holds with probability at least $1-\delta$ over the randomness in $\mathcal{H}_t$:*

$$V_t \le \left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^t V_0 + \left(\frac{5\sqrt{\alpha}\sigma^2}{\sqrt{\mu}} + \frac{80\Delta^2}{\alpha}\right)\ln\frac{eT}{\delta}. \tag{30}$$

Proof of Lemma C.5. We will invoke Lemma A.1 to show the results. To apply Lemma A.1, we first need to show the following two facts:

$$\text{Fact (I)}: \quad \sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \le \sqrt{V_t} \qquad \& \qquad \text{Fact (II)}: \quad \frac{1+\sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t - w_t\| \le \sqrt{V_t}. \tag{31}$$

Fact (I) verification. Since ϕ_t is μ-strongly convex and matrix $\mathbf{P}$ is PSD, then

$$\begin{aligned}
V_t &= \theta_t^\top \mathbf{P}\theta_t + \phi_t(w_t) - \phi_t(w_t^*) \ge \phi_t(w_t) - \phi_t(w_t^*) \\
&\ge \frac{\mu}{2}\|w_t - w_t^*\|^2 \qquad \Longrightarrow \qquad \sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \le \sqrt{V_t}.
\end{aligned}$$

Fact (II) verification. By definition of matrix $\mathbf{P}$ and simple calculation we have

$$\begin{aligned}
\sqrt{V_t} &\ge \sqrt{\theta_t^\top \mathbf{P}\theta_t} = \sqrt{\frac{1}{2\alpha}}\|(w_t - w_t^*) + (\sqrt{\mu\alpha} - 1)(w_{t-1} - w_t^*)\| \\
&= \sqrt{\frac{1}{2\alpha}}\|(1-\sqrt{\mu\alpha})(w_t - w_{t-1}) + \sqrt{\mu\alpha}(w_t - w_t^*)\| \\
&\ge \sqrt{\frac{1}{2\alpha}}(1-\sqrt{\mu\alpha})\|w_t - w_{t-1}\| - \sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \\
&\ge \sqrt{\frac{1}{2\alpha}}(1-\sqrt{\mu\alpha})\|w_t - w_{t-1}\| - \sqrt{V_t}.
\end{aligned}$$

Rearrange the above inequality, and recall the update rule of stochastic Nesterov accelerated gradient method, we have

$$\|z_t - w_t\| = \gamma\|w_t - w_{t-1}\| \le \frac{2\gamma\sqrt{2\alpha}}{1-\sqrt{\mu\alpha}}\sqrt{V_t} = \frac{2\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\sqrt{V_t},$$

where for the last equality we use the definition of γ as in (10). Rearrange it gives (31).

By Lemma C.3 and the choice of $\alpha \le 1/L$, we have

$$\begin{aligned}
V_{t+1} \le \left(1 - \frac{\sqrt{\mu\alpha}}{2}\right)V_t + \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\Bigg[&\sqrt{2\mu}\alpha(1-L\alpha)\langle u_{t,1}, -\varepsilon_t\rangle\sqrt{\frac{\mu}{2}}\|w_t - w_t^*\| \\
&+ \frac{2\mu\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\langle u_{t,2}, -\varepsilon_t\rangle\frac{1+\sqrt{\mu\alpha}}{2\sqrt{2\alpha}}\|z_t - w_t\| + \alpha\|\varepsilon_t\|^2\Bigg] + \frac{20\mu\Delta_t^2}{\sqrt{\mu\alpha}}.
\end{aligned} \tag{32}$$

Note that under Assumption C.2, there exists an absolute constant $c \geq 1$ such that for all $t \geq 0$, $\|\varepsilon_t\|^2$ is sub-exponential conditioned on $\mathcal{H}_t$ with parameter $c\sigma^2$, and ε_t is mean-zero sub-Gaussian conditioned on $\mathcal{H}_t$ with parameter $c\sigma$ [20, Theorem 30]. For convenience we simply let $c = 1$ here. Thus $\langle u_{t,1}, -\varepsilon_t\rangle$ is mean-zero sub-Gaussian conditioned on $\mathcal{H}_t$ with parameter σ, and Δ_t^2 is sub-exponential conditioned on $\mathcal{H}_t$ with parameter Δ^2 by assumption. Hence, in light of (32), we apply Lemma A.1 with

$$\mathcal{H}_t = \mathcal{H}_t, \quad V_t = V_t, \quad V'_{t,1} = \frac{\mu}{2}\|w_t - w_t^*\|^2, \quad V'_{t,2} = \frac{(1+\sqrt{\mu\alpha})^2}{8\alpha}\|z_t - w_t\|^2,$$

$$D_{t,1} = \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\sqrt{2\mu}\alpha(1-L\alpha)\langle u_{t,1}, -\varepsilon_t\rangle, \quad D_{t,2} = \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\frac{2\mu\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\langle u_{t,2}, -\varepsilon_t\rangle,$$

$$X_t = \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\alpha\|\varepsilon_t\|^2 + \frac{20\mu\Delta_t^2}{\sqrt{\mu\alpha}}, \quad \alpha_t = 1 - \frac{\sqrt{\mu\alpha}}{2}, \quad \kappa_t = 0,$$

$$\sigma_1 = \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\sqrt{2\mu}\alpha(1-L\alpha)\sigma, \quad \sigma_2 = \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\frac{2\mu\sqrt{2\alpha}}{1+\sqrt{\mu\alpha}}\alpha(1-L\alpha)\sigma,$$

$$\nu_t = \left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\alpha\sigma^2 + \frac{20\mu\Delta^2}{\sqrt{\mu\alpha}},$$

yielding the following recursion

$$\mathbb{E}[\exp(\lambda V_{t+1})] \leq \exp\left(\lambda\left[\left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\alpha\sigma^2 + \frac{20\mu\Delta^2}{\sqrt{\mu\alpha}}\right]\right)\mathbb{E}\left[\exp\left(\lambda\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)V_t\right)\right] \tag{33}$$

for all λ satisfying

$$0 \leq \lambda \leq \min\left\{\frac{2}{125\alpha\sqrt{\mu\alpha}\sigma^2}, \frac{1}{5\alpha\sigma^2/2 + 40\mu\Delta^2/\sqrt{\mu\alpha}}\right\}.$$

We then apply (33) recursively to deduce

$$\begin{aligned}\mathbb{E}[\exp(\lambda V_{t+1})] &\leq \exp\left[\lambda\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^t V_0 + \lambda\left(\left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\alpha\sigma^2 + \frac{20\mu\Delta^2}{\sqrt{\mu\alpha}}\right)\sum_{i=0}^{t-1}\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^i\right] \\ &\leq \exp\left\{\lambda\left[\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^t V_0 + 4\left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\frac{\alpha}{\sqrt{\mu\alpha}}\sigma^2 + \frac{80\Delta^2}{\alpha}\right]\right\}\end{aligned}$$

for all λ satisfying

$$0 \leq \lambda \leq \min\left\{\frac{2}{125\alpha\sqrt{\mu\alpha}\sigma^2}, \frac{1}{5\alpha\sigma^2/2 + 40\mu\Delta^2/\sqrt{\mu\alpha}}\right\}.$$

Moreover, setting

$$\nu := \frac{5\sqrt{\alpha}\sigma^2}{\sqrt{\mu}} + \frac{80\Delta^2}{\alpha}$$

and taking into account $\alpha \leq 1/25L$, then we have

$$4\left(1 + \frac{\sqrt{\mu\alpha}}{4}\right)\frac{\alpha}{\sqrt{\mu\alpha}}\sigma^2 + \frac{80\Delta^2}{\alpha} \leq \nu$$

and

$$\frac{1}{\nu} = \frac{1}{5\sqrt{\alpha}\sigma^2/\sqrt{\mu} + 80\Delta^2/\alpha} \leq \min\left\{\frac{2}{125\alpha\sqrt{\mu\alpha}\sigma^2}, \frac{1}{5\alpha\sigma^2/2 + 40\mu\Delta^2/\sqrt{\mu\alpha}}\right\}.$$

Thus we obtain

$$\mathbb{E}\left[\exp\left(\lambda\left(V_t - \left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^t V_0\right)\right)\right] \leq \exp(\lambda\nu) \quad \text{for all} \quad 0 \leq \lambda \leq 1/\nu.$$

Taking $\lambda = 1/\nu$ and applying Markov's inequality and union bound completes the proof. □

The following result shows the second part of Lemma 4.3.

Lemma C.6 (High-probability distance tracking, without drift)**.** *Under the same setting as in Lemma C.4 with $\alpha \le 1/25L$, for any given $\delta \in (0,1)$ and all $t \in [T]$, the following holds with probability at least $1-\delta$ over the randomness in $\mathcal{H}_t$:*

$$V_t \le \left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^t V_0 + \frac{5\sqrt{\alpha}\sigma^2}{\sqrt{\mu}} \ln \frac{eT}{\delta}. \tag{34}$$

Proof of Lemma C.6. First it is easy to verify that

$$\frac{1}{L}\sqrt{\frac{\mu}{2}}\|\nabla\phi_t(w_t) - \nabla\phi_t(w^*)\| \le \sqrt{V_t} \qquad \text{and} \qquad \frac{1+\sqrt{\mu\alpha}}{2L\sqrt{2\alpha}}\|\nabla\phi_t(z_t) - \nabla\phi_t(w_t)\| \le \sqrt{V_t}.$$

Then we apply Lemma A.1 to obtain the final result. We omit the detailed proof here since it follows the same procedure as in proof of Lemma C.5. □

D Proofs of Results in Section 4.3.2

We first present the following algebraic fact under suitable choice of parameters.

Lemma D.1 (Parameter choice, informal)**.** *For any given $\delta \in (0,1)$ and any small ϵ satisfying*

$$\epsilon \le \left(\frac{170 \cdot 32 e d_0 L_0^2 \tilde{\sigma}_{g,1}^2}{\delta\mu^2} \max\left\{\frac{l_{g,1}}{\tilde{\sigma}_{g,1}}, \frac{\bar{\sigma}}{d_0}\right\}\right)^{1/3}, \tag{35}$$

if we set parameters α, β, η, T as

$$1-\beta = \frac{\mu^2\epsilon^2}{170 \cdot 64 L_0^2 \tilde{\sigma}_{g,1}^2 \ln(P)}, \quad \eta = \min\left\{\frac{\tilde{\sigma}_{g,1}}{l_{g,1}}, \frac{d_0}{\bar{\sigma}}\right\}(1-\beta), \quad \alpha = \frac{1}{\mu}(1-\beta), \quad \sigma_{g,1} = \sqrt{\mu\alpha}\tilde{\sigma}_{g,1}, \quad T = \frac{4d_0}{\eta\epsilon}, \tag{36}$$

where $\bar{\sigma}$ is defined in Lemma B.4, and d_0 and P are defined as

$$d_0 = \Phi(x_0) - \inf_{x\in\mathbb{R}^{d_x}} \Phi(x), \quad P = \left(\frac{170 \cdot 64 e d_0 L_0^2 \tilde{\sigma}_{g,1}^2}{\delta\mu^2\epsilon^3} \max\left\{\frac{l_{g,1}}{\tilde{\sigma}_{g,1}}, \frac{\bar{\sigma}}{d_0}\right\}\right)^2. \tag{37}$$

Then the following holds for all $t \in [T]$:

$$\left(\frac{4\alpha\tilde{\sigma}_{g,1}^2}{\mu} + \frac{160\eta^2 l_{g,1}^2}{\mu^3\alpha}\right) \ln\frac{eT}{\delta} \le \frac{\epsilon^2}{64L_0^2}.$$

Proof of Lemma D.1. By Lemma B.1, we have $\Delta_t = \|y_t^* - y_{t+1}^*\| \le \frac{l_{g,1}}{\mu}\|x_t - x_{t+1}\| = \eta l_{g,1}/\mu$. Thus in our bilevel setting, we choose $\Delta = \eta l_{g,1}/\mu$, where Δ is defined in Section 4.3.1. By choice of α, η, T as in (36), we have

$$\begin{aligned}\left(\frac{10\alpha\tilde{\sigma}_{g,1}^2}{\mu} + \frac{160\eta^2 l_{g,1}^2}{\mu^3\alpha}\right) \ln\frac{eT}{\delta} &= \left(\frac{10(1-\beta)\tilde{\sigma}_{g,1}^2}{\mu^2} + \frac{160\eta^2 l_{g,1}^2}{\mu^2(1-\beta)}\right) \ln\left(\frac{4ed_0}{\delta\eta\epsilon}\right) \\ &\le \frac{170(1-\beta)\tilde{\sigma}_{g,1}^2}{\mu^2} \ln\left(\frac{4ed_0}{\delta\epsilon(1-\beta)} \max\left\{\frac{l_{g,1}}{\tilde{\sigma}_{g,1}}, \frac{\bar{\sigma}}{4d_0}\right\}\right).\end{aligned}$$

Now we choose β to be

$$1-\beta = \frac{\mu^2\epsilon^2}{170 \cdot 64 L_0^2 \tilde{\sigma}_{g,1}^2 \ln(P)}, \quad \text{where} \quad P = \left(\frac{170 \cdot 64 e d_0 L_0^2 \tilde{\sigma}_{g,1}^2}{\delta\mu^2\epsilon^3} \max\left\{\frac{l_{g,1}}{\tilde{\sigma}_{g,1}}, \frac{\bar{\sigma}}{d_0}\right\}\right)^2.$$

Then we have

$$\frac{170(1-\beta)\tilde{\sigma}_{g,1}^2}{\mu^2} \ln\left(\frac{4ed_0 l_{g,1}}{\delta\epsilon\tilde{\sigma}_{g,1}(1-\beta)}\right) = \frac{\epsilon^2}{64L_0^2\ln(P)} \ln\left(\sqrt{P}\ln(P)\right) \le \frac{\epsilon^2}{64L_0^2},$$

where we use the fact that $\ln(\sqrt{P}\ln(P)) \le \ln(P) \le \ln^2(P)$ for any $P \ge 4$ by choice of ϵ as in (35). □

In the rest of this section, we assume Assumptions 3.1 to 3.4 hold. In addition, the failure probability $\delta \in (0,1)$ and $\epsilon > 0$ are chosen in the same way as in Theorem 4.1.

D.1 Proof of Lemma 4.4

Lemma D.2 (Warm-start, Restatement of Lemma 4.4)**.** *Let $\{y_t^{\text{init}}\}$ be the iterates produced by line 2 of Algorithm 2. Set $\alpha^{\text{init}} = \mu\alpha^2 = \widetilde{\Theta}(\epsilon^4)$ with α defined in* (36)*, $\sigma_{g,1} = (\mu\alpha)^{1/4}\tilde{\sigma}_{g,1}$, and $\phi_t(y) \equiv g(x_0, y)$. Then $\|y_{T_0}^{\text{init}} - y_0^*\| \leq \sqrt{\frac{\mu\alpha}{32}}\frac{\epsilon}{L_0}$ holds with probability at least $1-\delta$ over the randomness in $\widetilde{\mathcal{F}}^{\text{init}}$ (we denote this event as $\mathcal{E}_{\text{init}}$) in $T_0 = \widetilde{O}(\epsilon^{-2})$ iterations, where*

$$T_0 = \ln\left(\frac{\mu^3\alpha^3\epsilon^2}{256L_0^2\|y_0^{\text{init}} - y_0^*\|^2}\right) \Big/ \ln\left(1 - \frac{\mu\alpha}{4}\right) = \widetilde{O}(\epsilon^{-2}). \tag{38}$$

Proof of Lemma D.2. By Lemmas C.6 and D.1 and μ-strong convexity of g in y, we have with probability at least $1-\delta$ over the randomness in $\mathcal{F}^{\text{init}}$ that

$$\begin{aligned}
\|y_{T_0}^{\text{init}} - y_0^*\|^2 &\leq \frac{2}{\mu}\left(1 - \frac{\sqrt{\mu^2\alpha^2}}{4}\right)^{T_0} U_0^{\text{init}} + \frac{10\mu\alpha^2\tilde{\sigma}_{g,1}^2}{\mu}\ln\frac{eT_0}{\delta} \\
&\leq \frac{2}{\mu}\left(1 - \frac{\mu\alpha}{4}\right)^{T_0} U_0^{\text{init}} + \frac{\mu\alpha\epsilon^2}{64L_0^2},
\end{aligned}$$

where the first inequality uses the choice of $\alpha^{\text{init}} = \mu\alpha^2$. By $l_{g,1}$-smoothness of g we have

$$\begin{aligned}
U_0^{\text{init}} &\leq \frac{2 - \sqrt{\mu^2\alpha^2} + \mu^2\alpha^2}{2\mu\alpha^2}\|y_0^{\text{init}} - y_0^*\|^2 + g(x_0, y_0^{\text{init}}) - g(x_0, y_0^*) \\
&\leq \frac{3}{2\mu\alpha^2}\|y_0^{\text{init}} - y_0^*\|^2 + \frac{l_{g,1}}{2}\|y_0^{\text{init}} - y_0^*\|^2 \leq \frac{2}{\mu\alpha^2}\|y_0^{\text{init}} - y_0^*\|^2,
\end{aligned}$$

where the last inequality uses $\alpha \leq 1/l_{g,1}$. Now we set

$$\frac{2}{\mu}\left(1 - \frac{\mu\alpha}{4}\right)^{T_0}\frac{2}{\mu\alpha^2}\|y_0^{\text{init}} - y_0^*\|^2 + \frac{\mu\alpha\epsilon^2}{64L_0^2} \leq \frac{\mu\alpha\epsilon^2}{32L_0^2},$$

which gives

$$T_0 \geq \ln\left(\frac{\mu^3\alpha^3\epsilon^2}{256L_0^2\|y_0^{\text{init}} - y_0^*\|^2}\right) \Big/ \ln\left(1 - \frac{\mu\alpha}{4}\right).$$

By choice of α as in (36) and simple calculation we obtain $T_0 = \widetilde{O}(\epsilon^{-2})$ when ϵ is small. □

D.2 Proof of Lemma 4.5

Lemma D.3 (Option I, Restatement of Lemma 4.5)**.** *Under event $\mathcal{E}_{\text{init}}$, let $\{y_t\}$ be the iterates produced by Option I. Set $\alpha = \widetilde{\Theta}(\epsilon^2)$ as in* (36)*, $\sigma_{g,1} = (\mu\alpha)^{1/4}\tilde{\sigma}_{g,1}$, and $\phi_t(y) = g(x_t, y) = \frac{\mu}{2}\|y - y_t^*\|^2$. Then for any $t \in [T]$, Algorithm 2 guarantees with probability at least $1-\delta$ over the randomness in $\widetilde{\mathcal{F}}_T^1$ (we denote this event as $\mathcal{E}_y^1$) that $\|y_t - y_t^*\| \leq \epsilon/2L_0$.*

Proof of Lemma D.3. By Lemmas C.5 and D.2 we have

$$\begin{aligned}
\|y_t - y_t^*\|^2 &\leq \frac{2}{\mu}\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^t U_0 + \left(\frac{10\alpha\tilde{\sigma}_{g,1}^2}{\mu} + \frac{160\eta^2 l_{g,1}^2}{\mu^3\alpha}\right)\ln\frac{eT}{\delta} \\
&\leq \frac{2}{\mu}\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^t \frac{2}{\alpha}\|y_{T_0}^{\text{init}} - y_0^*\|^2 + \left(\frac{10\alpha\tilde{\sigma}_{g,1}^2}{\mu} + \frac{160\eta^2 l_{g,1}^2}{\mu^3\alpha}\right)\ln\frac{eT}{\delta} \\
&\leq \frac{4}{\mu\alpha}\|y_{T_0}^{\text{init}} - y_0^*\|^2 + \frac{\epsilon^2}{64L_0^2} \leq \frac{\epsilon^2}{4L_0^2}.
\end{aligned}$$

Thus we conclude that for all $t \in [T]$, we have $\|y_t - y_t^*\| \leq \epsilon/2L_0$. □

D.3 Proof of Lemma 4.6

Lemma D.4 (Option II, Restatement of Lemma 4.6)**.** *Under event $\mathcal{E}_{\text{init}}$, let $\{y_t\}$ be the iterates produced by Option II. Set $\alpha = \widetilde{\Theta}(\epsilon^2)$ as in* (36)*, $\sigma_{g,1} = (\mu\alpha)^{1/4}\tilde{\sigma}_{g,1}$, and run SNAG in each update round for*

$$N = \ln\left(\frac{\mu\alpha}{128}\right) \Big/ \ln\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right) = \widetilde{O}(\epsilon^{-1})$$

steps in every $I = \frac{\mu\epsilon}{2(1-\beta)L_0\tilde{\sigma}_{g,1}} = \widetilde{O}(\epsilon^{-1})$ iterations, set $\phi_t(y) = g(x_t, y)$ when t is a multiple of I (i.e., x_t is fixed for each update round of Option II so g can be general functions). Then for any $t \in [T]$, Algorithm 2 guarantees with probability at least $1-\delta$ over the randomness in $\sigma(\cup_{t\le T}\widetilde{\mathcal{F}}_t^2)$ (we denote this event as $\mathcal{E}_y^2$) that $\|y_t - y_t^*\| \le \epsilon/L_0$.

Proof of Lemma D.4. At the beginning of the first round, by Lemmas D.2 and D.3 we have $\|y_0 - y_0^*\| \le \epsilon/2L_0$, then we do not update the lower-level variable until $t = I$-th iteration, then for $t = I$, we have

$$\begin{aligned}\|y_I - y_I^*\| = \|y_0 - y_I^*\| &\le \|y_0 - y_0^*\| + \sum_{i=1}^{I}\|y_i^* - y_{i-1}^*\| \\ &\le \frac{\epsilon}{2L_0} + \frac{\eta l_{g,1}}{\mu} I = \frac{\epsilon}{L_0},\end{aligned}$$

where in the last equality we plug in the definition of η and I. By $l_{g,1}$-smoothness of g we have

$$\begin{aligned}U_I &\le \frac{2 - 2\sqrt{\mu\alpha} + \mu\alpha}{2\alpha}\|y_I - y_0^*\|^2 + g(x_I, y_I) - g(x_I, y_I^*) \\ &\le \frac{3}{2\alpha}\|y_I - y_I^*\|^2 + \frac{l_{g,1}}{2}\|y_I - y_I^*\|^2 \le \frac{2\epsilon^2}{\alpha L_0^2}\end{aligned}$$

Then for N steps update in the inner loops of $t = I$-th iteration, we set

$$\frac{2}{\mu}\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^N \frac{2\epsilon^2}{\alpha L_0^2} + \frac{\epsilon^2}{64L_0^2} \le \frac{\epsilon^2}{16L_0^2},$$

which gives

$$N \ge \ln\left(\frac{\mu\alpha}{128}\right) \Big/ \ln\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)$$

By choice of α as in (36) and simple calculation we obtain $N = \widetilde{O}(\epsilon^{-1})$ when ϵ is small. Now we have

$$\|y_{I+1} - y_I^*\|^2 = \|y_I^N - y_I^*\|^2 \le \frac{2}{\mu}\left(1 - \frac{\sqrt{\mu\alpha}}{4}\right)^N \frac{2\epsilon^2}{\alpha L_0^2} + \frac{\epsilon^2}{64L_0^2} \le \frac{\epsilon^2}{16L_0^2},$$

which yields

$$\|y_{I+1} - y_{I+1}^*\| \le \|y_{I+1} - y_I^*\| + \|y_I^* - y_{I+1}^*\| \le \frac{\epsilon}{4L_0} + \frac{\eta l_{g,1}}{\mu} \le \frac{\epsilon}{2L_0},$$

where we choose $1-\beta$ to be small (see (56) for details) such that η is small enough to make above inequality holds. Repeating the same process yields the result. □

D.4 Proof of Lemma 4.7

Lemma D.5 (Averaging, Restatement of Lemma 4.7)**.** *Under Assumptions 3.1 to 3.4 and event $\mathcal{E}_{\text{init}} \cap \mathcal{E}_y^1$ (Option I) or $\mathcal{E}_{\text{init}} \cap \mathcal{E}_y^2$ (Option II), we further set $\tau = \sqrt{\mu\alpha}$ in the averaging step (line 21 of Algorithm 2). Then for any $t \ge 0$ we have*

$$\|\hat{y}_t - y_t^*\| \le \frac{2\epsilon}{L_0} \quad \textit{and} \quad \|\hat{y}_{t+1} - \hat{y}_t\| \le \frac{\mu\epsilon^2}{24L_0^2\tilde{\sigma}_{g,1}} =: \vartheta.$$

Proof of Lemma D.5. We will first show the following result by induction, i.e., for any $t \geq 0$, the averaged sequence $\{\hat{y}_t\}$ satisfies

$$\|\hat{y}_t - y_t^*\| \leq \frac{(1-\tau)\eta l_{g,1}}{\tau\mu} + \frac{\epsilon}{L_0}. \tag{39}$$

For $t = 0$, by Lemma D.2 we have

$$\|\hat{y}_0 - y_0^*\| = \|y_{T_0}^{\text{init}} - y_0^*\| \leq \sqrt{\frac{\mu\alpha}{32}}\frac{\epsilon}{L_0} = \sqrt{\frac{1-\beta}{32}}\frac{\epsilon}{L_0} \leq \frac{\epsilon}{L_0},$$

thus the base case holds. Now suppose (39) holds for some $t \geq 0$, then for time step $t+1$ we have

$$\begin{aligned}
\|\hat{y}_{t+1} - y_{t+1}^*\| &= \|(1-\tau)(\hat{y}_t - y_{t+1}^*) + \tau(y_{t+1} - y_{t+1}^*)\| \\
&= \|(1-\tau)(\hat{y}_t - y_t^*) + (1-\tau)(y_t^* - y_{t+1}^*) + \tau(y_{t+1} - y_{t+1}^*)\| \\
&\leq (1-\tau)\|\hat{y}_t - y_t^*\| + (1-\tau)\|y_t^* - y_{t+1}^*\| + \tau\|y_{t+1} - y_{t+1}^*\| \\
&\leq (1-\tau)\left(\frac{(1-\tau)\eta l_{g,1}}{\tau\mu} + \frac{\epsilon}{L_0}\right) + \frac{(1-\tau)\eta l_{g,1}}{\mu} + \frac{\tau\epsilon}{L_0} \\
&\leq \frac{(1-\tau)\eta l_{g,1}}{\tau\mu} + \frac{\epsilon}{L_0},
\end{aligned}$$

where we use induction hypothesis in the second inequality. Therefore, we have that (39) holds for any $t \geq 0$. Also, as a consequence, for any $t \geq 0$ we have

$$\begin{aligned}
\|\hat{y}_{t+1} - \hat{y}_t\| &= \|\tau(y_{t+1} - \hat{y}_t)\| \\
&\leq \tau\|y_{t+1} - y_{t+1}^*\| + \tau\|y_{t+1}^* - y_t^*\| + \tau\|y_t^* - \hat{y}_t\| \\
&\leq \tau\left(\frac{\epsilon}{L_0} + \frac{\eta l_{g,1}}{\mu} + \frac{(1-\tau)\eta l_{g,1}}{\tau\mu} + \frac{\epsilon}{L_0}\right) \\
&= \tau\left(\frac{\eta l_{g,1}}{\tau\mu} + \frac{2\epsilon}{L_0}\right).
\end{aligned}$$

Now we plug in the definition of $\alpha, \beta, \tau, \eta$ as in (36) to obtain

$$\|\hat{y}_t - y_t^*\| \leq \frac{(1-\tau)\eta l_{g,1}}{\tau\mu} + \frac{\epsilon}{L_0} = \frac{\tilde{\sigma}_{g,1}}{\mu}\sqrt{1-\beta} + \frac{\epsilon}{L_0} \leq \frac{2\epsilon}{L_0}$$

and

$$\|\hat{y}_{t+1} - \hat{y}_t\| \leq \tau\left(\frac{\eta l_{g,1}}{\tau\mu} + \frac{2\epsilon}{L_0}\right) \leq \frac{\mu\epsilon^2}{24L_0^2\tilde{\sigma}_{g,1}}.$$

□

D.5 Proof of Lemma 4.8

Lemma D.6 (Restatement of Lemma 4.8)**.** *Under Assumptions 3.1 to 3.4 and event $\mathcal{E}_{\text{init}} \cap \mathcal{E}_y^1$ (Option I) or $\mathcal{E}_{\text{init}} \cap \mathcal{E}_y^2$ (Option II), define $\epsilon_t = m_t - \mathbb{E}_t[\bar{\nabla} f(x_t, \hat{y}_t; \bar{\xi}_t)]$, then we have the following averaged cumulative error bound:*

$$\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\epsilon_t\| \leq \frac{\bar{\sigma}}{T(1-\beta)} + \sqrt{1-\beta}\bar{\sigma} + \frac{\bar{L}_0}{\sqrt{1-\beta}}\sqrt{\frac{2(\eta^2+\vartheta^2)}{S}} + \bar{L}_1\sqrt{\frac{2(\eta^2+\vartheta^2)}{S(1-\beta)}}\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\nabla\Phi(x_t)\|.$$

Proof of Lemma D.6. Define $\epsilon_t = m_t - \mathbb{E}_t[\bar{\nabla} f(x_t, \hat{y}_t; \bar{\xi}_t)]$, also define $\tilde{\epsilon}_t$ and $\hat{\epsilon}_t$ as

$$\begin{aligned}
\tilde{\epsilon}_t &= \bar{\nabla} f(x_t, \hat{y}_t; \bar{\xi}_t) - \mathbb{E}_t[\bar{\nabla} f(x_t, \hat{y}_t; \bar{\xi}_t)], \\
\hat{\epsilon}_t &= \bar{\nabla} f(x_t, \hat{y}_t; \bar{\xi}_t) - \bar{\nabla} f(x_{t-1}, \hat{y}_{t-1}; \bar{\xi}_t) - \mathbb{E}_t[\bar{\nabla} f(x_t, \hat{y}_t; \bar{\xi}_t)] + \mathbb{E}_t[\bar{\nabla} f(x_{t-1}, \hat{y}_{t-1}; \bar{\xi}_t)].
\end{aligned}$$

By definition of ϵ_t, $\tilde{\epsilon}_t$ and $\hat{\epsilon}_t$, we have the following recursion for any $t \geq 0$:

$$\epsilon_{t+1} = \beta\epsilon_t + (1-\beta)\hat{\epsilon}_{t+1} + \beta\tilde{\epsilon}_{t+1}. \tag{40}$$

Then we apply (40) recursively to obtain

$$\epsilon_t = \beta^t \epsilon_0 + \beta \sum_{i=1}^{t} \beta^{t-i} \tilde{\epsilon}_i + (1-\beta) \sum_{i=1}^{t} \beta^{t-i} \hat{\epsilon}_i,$$

which by triangle inequality and total expectation gives

$$\mathbb{E}\|\epsilon_t\| = \beta^t \underbrace{\mathbb{E}\|\epsilon_0\|}_{Err_1} + (1-\beta) \underbrace{\mathbb{E}\left\|\sum_{i=1}^{t} \beta^{t-i} \hat{\epsilon}_i\right\|}_{Err_2} + \beta \underbrace{\mathbb{E}\left\|\sum_{i=1}^{t} \beta^{t-i} \tilde{\epsilon}_i\right\|}_{Err_3}. \tag{41}$$

Bounding Err_1. By definition of ϵ_0 and Lemma B.4, along with Jensen's inequality, we have

$$\mathbb{E}\|\epsilon_0\| \leq \sqrt{\mathbb{E}\|\epsilon_0\|^2} \leq \bar{\sigma}. \tag{42}$$

Bounding Err_2. We apply Lemma B.4 and follow the similar procedure as in [38, Lemma D.9] to obtain

$$\mathbb{E}\left\|\sum_{i=1}^{t} \beta^{t-i} \tilde{\epsilon}_i\right\| \leq \sqrt{\mathbb{E}\left\|\sum_{i=1}^{t} \beta^{t-i} \tilde{\epsilon}_i\right\|^2} \leq \sqrt{\sum_{i=1}^{t} \beta^{2(t-i)} \mathbb{E}\|\tilde{\epsilon}_i\|^2} \leq \frac{\bar{\sigma}}{\sqrt{1-\beta}}, \tag{43}$$

where we use Jensen's inequality for the first step.

Bounding Err_3. We will first use induction to show that for $0 \leq i \leq t+1$, the following inequality holds:

$$\mathbb{E}\left[\left\|\sum_{j=1}^{t} \beta^{t-j} \hat{\epsilon}_j\right\|\right] \leq \sqrt{\frac{2(\eta^2+\vartheta^2)}{S}} \bar{L}_1 \sum_{j=t+1-i}^{t} \beta^{t-j} \mathbb{E}\|\nabla\Phi(x_j)\| + \mathbb{E}\left[\sqrt{\frac{2(\eta^2+\vartheta^2)\bar{L}_0^2}{S} \sum_{j=1}^{i} \beta^{2j-2} + \left\|\sum_{j=1}^{t-i} \beta^{t-j} \hat{\epsilon}_j\right\|^2}\right]. \tag{44}$$

Then it's easy to check that by setting $i = t+1$ we can obtain the bound. When $i = 0$, (44) holds obviously since

$$\mathbb{E}\left[\left\|\sum_{j=1}^{t} \beta^{t-j} \hat{\epsilon}_j\right\|\right] \leq \mathbb{E}\left[\sqrt{\left\|\sum_{j=1}^{t} \beta^{t-j} \hat{\epsilon}_j\right\|^2}\right] = \mathbb{E}\left[\left\|\sum_{j=1}^{t} \beta^{t-j} \hat{\epsilon}_j\right\|\right].$$

Hence the base case stands. Now suppose (44) holds for some $i \geq 0$, and we aim to show that (44) holds for $i+1$. In fact, we have

$$\mathbb{E}\left[\sqrt{\frac{2(\eta^2+\vartheta^2)\bar{L}_0^2}{S}\sum_{j=1}^{i}\beta^{2j-2}+\left\|\sum_{j=1}^{t-i}\beta^{t-j}\hat{\epsilon}_j\right\|^2}\right] \tag{45}$$

$$=\mathbb{E}_{\mathcal{F}_{t-i-1}}\left[\mathbb{E}_{t-i-1}\left[\sqrt{\frac{2(\eta^2+\vartheta^2)\bar{L}_0^2}{S}\sum_{j=1}^{i}\beta^{2j-2}+\left\|\sum_{j=1}^{t-i}\beta^{t-j}\hat{\epsilon}_j\right\|^2}\right]\right] \tag{46}$$

$$\leq \mathbb{E}_{\mathcal{F}_{t-i-1}}\left[\mathbb{E}_{t-i-1}\sqrt{\left[\frac{2(\eta^2+\vartheta^2)\bar{L}_0^2}{S}\sum_{j=1}^{i}\beta^{2j-2}+\left\|\sum_{j=1}^{t-i}\beta^{t-j}\hat{\epsilon}_j\right\|^2\right]}\right] \tag{47}$$

$$=\mathbb{E}_{\mathcal{F}_{t-i-1}}\left[\mathbb{E}_{t-i-1}\sqrt{\left[\frac{2(\eta^2+\vartheta^2)\bar{L}_0^2}{S}\sum_{j=1}^{i}\beta^{2j-2}+\beta^{2i}\|\hat{\epsilon}_{t-i}\|^2+\left\|\sum_{j=1}^{t-i-1}\beta^{t-j}\hat{\epsilon}_j\right\|^2\right]}\right] \tag{48}$$

$$\leq \mathbb{E}_{\mathcal{F}_{t-i-1}}\left[\mathbb{E}_{t-i-1}\sqrt{\left[\frac{2(\eta^2+\vartheta^2)\bar{L}_0^2}{S}\sum_{j=1}^{i}\beta^{2j-2}+\frac{\beta^{2i}}{S}2(\bar{L}_0^2+\bar{L}_1^2\|\nabla\Phi(x_{t-i})\|^2)(\eta^2+\vartheta^2)+\left\|\sum_{j=1}^{t-i-1}\beta^{t-j}\hat{\epsilon}_j\right\|^2\right]}\right] \tag{49}$$

$$=\mathbb{E}_{\mathcal{F}_{t-i-1}}\left[\sqrt{\frac{2\beta^{2i}}{S}\bar{L}_1^2(\eta^2+\vartheta^2)\|\nabla\Phi(x_{t-i})\|^2+\frac{2(\eta^2+\vartheta^2)\bar{L}_0^2}{S}\sum_{j=1}^{i+1}\beta^{2j-2}+\left\|\sum_{j=1}^{t-i-1}\beta^{t-j}\hat{\epsilon}_j\right\|^2}\right] \tag{50}$$

$$\leq \mathbb{E}_{\mathcal{F}_{t-i-1}}\left[\sqrt{\frac{2(\eta^2+\vartheta^2)}{S}}\beta^i\bar{L}_1\|\nabla\Phi(x_{t-i})\|+\sqrt{\frac{2(\eta^2+\vartheta^2)\bar{L}_0^2}{S}\sum_{j=1}^{i+1}\beta^{2j-2}+\left\|\sum_{j=1}^{t-i-1}\beta^{t-j}\hat{\epsilon}_j\right\|^2}\right], \tag{51}$$

where (46) follows by law of total expectation, (47) follows by Jensen's inequality, (48) uses the fact that $\hat{\epsilon}_j$ for $j < t-i$ are $\mathcal{F}_{t-i-1}$-measurable, and are uncorrelated with $\hat{\epsilon}_{t-i}$; for (49) we use Lemmas B.6 and D.5 to derive

$$\begin{aligned}
\mathbb{E}_{t-i-1}[\|\hat{\epsilon}_{t-i}\|^2] &= \mathbb{E}_{t-i-1}\left[\|\bar{\nabla}f(x_{t-i},\hat{y}_{t-i};\bar{\xi}_{t-i})-\bar{\nabla}f(x_{t-i-1},\hat{y}_{t-i-1};\bar{\xi}_{t-i})\right.\\
&\quad\left.-\mathbb{E}_{t-i}[\bar{\nabla}f(x_{t-i},\hat{y}_{t-i};\bar{\xi}_{t-i})]+\mathbb{E}_{t-i}[\bar{\nabla}f(x_{t-i-1},\hat{y}_{t-i-1};\bar{\xi}_{t-i})]\|^2\right]\\
&\leq \mathbb{E}_{t-i-1}\left[\|\bar{\nabla}f(x_{t-i},\hat{y}_{t-i};\bar{\xi}_{t-i})-\bar{\nabla}f(x_{t-i-1},\hat{y}_{t-i-1};\bar{\xi}_{t-i})\|^2\right]\\
&\leq 2\mathbb{E}_{t-i-1}\left[\|\bar{\nabla}f(x_{t-i},\hat{y}_{t-i};\bar{\xi}_{t-i})-\bar{\nabla}f(x_{t-i},\hat{y}_{t-i-1};\bar{\xi}_{t-i})\|^2\right]\\
&\quad+2\mathbb{E}_{t-i-1}\left[\|\bar{\nabla}f(x_{t-i},\hat{y}_{t-i-1};\bar{\xi}_{t-i})-\bar{\nabla}f(x_{t-i-1},\hat{y}_{t-i-1};\bar{\xi}_{t-i})\|^2\right]\\
&\leq \frac{2}{S}(\bar{L}_0^2+\bar{L}_1^2\|\nabla\Phi(x_{t-i})\|^2)(\|\hat{y}_{t-i}-\hat{y}_{t-i-1}\|^2+\|x_{t-i}-x_{t-i-1}\|^2)\\
&= \frac{2}{S}(\bar{L}_0^2+\bar{L}_1^2\|\nabla\Phi(x_{t-i})\|^2)(\eta^2+\vartheta^2).
\end{aligned}$$

And (50) follows from the fact that x_{t-i} is $\mathcal{F}_{t-i-1}$-measurable, (51) uses $\sqrt{a+b}\leq\sqrt{a}+\sqrt{b}$ for $a,b\geq 0$. Hence the induction proof is completed. We set $i=t+1$ to obtain

$$\begin{aligned}
\mathbb{E}\left[\left\|\sum_{i=1}^{t}\beta^{t-i}\hat{\epsilon}_i\right\|\right] &\leq \sqrt{\frac{2(\eta^2+\vartheta^2)}{S}}\bar{L}_1\sum_{i=0}^{t}\beta^{t-i}\mathbb{E}\|\nabla\Phi(x_i)\|+\sqrt{\frac{2(\eta^2+\vartheta^2)\bar{L}_0^2}{S}\sum_{i=0}^{t}\beta^{2i}}\\
&\leq \sqrt{\frac{2(\eta^2+\vartheta^2)}{S}}\bar{L}_1\sum_{i=0}^{t}\beta^{t-i}\mathbb{E}\|\nabla\Phi(x_i)\|+\frac{\bar{L}_0}{\sqrt{1-\beta}}\sqrt{\frac{2(\eta^2+\vartheta^2)}{S}}.
\end{aligned} \tag{52}$$

Final Bound. Combining (42), (43) and (52) yields

$$\mathbb{E}\|\epsilon_t\|\leq\beta^t\bar{\sigma}+\sqrt{1-\beta}\bar{\sigma}+\frac{\bar{L}_0}{\sqrt{1-\beta}}\sqrt{\frac{2(\eta^2+\vartheta^2)}{S}}+\sqrt{\frac{2(\eta^2+\vartheta^2)}{S}}\bar{L}_1\sum_{i=0}^{t}\beta^{t-i}\mathbb{E}\|\nabla\Phi(x_i)\|.$$

Taking summation and dividing $1/T$ on both sides gives the final result

$$\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\epsilon_t\| \le \frac{\bar{\sigma}}{T(1-\beta)} + \sqrt{1-\beta}\bar{\sigma} + \frac{\bar{L}_0}{\sqrt{1-\beta}}\sqrt{\frac{2(\eta^2+\vartheta^2)}{S}} + \bar{L}_1\sqrt{\frac{2(\eta^2+\vartheta^2)}{S(1-\beta)}}\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\nabla\Phi(x_t)\|.$$

□

E Proof of Theorem 4.1

Before starting the proof of main results, i.e., Theorem 4.1, we first need the following lemma.

Lemma E.1. *Suppose that Assumptions 3.1 to 3.4 hold. For any η satisfying*

$$\eta \le \frac{1}{\sqrt{2(1+l_{g,1}^2/\mu^2)(L_{x,1}^2+L_{y,1}^2)}},$$

it holds that

$$\begin{aligned}
&\left(1-\frac{1}{2}\eta L_1 - 2L_1\|\hat{y}_t - y_t^*\|\right)\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\nabla\Phi(x_t)\| \\
&\le \frac{\Phi(x_0)-\Phi(x_T)}{T\eta} + \frac{2}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\epsilon_t\| + \frac{2l_{g,1}l_{f,0}}{\mu}\left(1-\frac{\mu}{l_{g,1}}\right)^Q + \frac{2L_0}{T}\sum_{t=0}^{T-1}\|\hat{y}_t - y_t^*\| + \frac{1}{2}\eta L_0.
\end{aligned}$$

Proof of Lemma E.1. Define $h_t = m_t - \nabla\Phi(x_t)$. Then we apply Lemma B.3 to obtain

$$\begin{aligned}
\Phi(x_{t+1}) &\le \Phi(x_t) + \langle\nabla\Phi(x_t), x_{t+1}-x_t\rangle + \frac{L_0 + L_1\|\nabla\Phi(x_t)\|}{2}\|x_{t+1}-x_t\|^2 \\
&= \Phi(x_t) - \eta\langle\nabla\Phi(x_t), \frac{m_t}{\|m_t\|}\rangle + \frac{1}{2}\eta^2(L_0 + L_1\|\nabla\Phi(x_t)\|) \\
&= \Phi(x_t) - \eta\langle m_t - h_t, \frac{m_t}{\|m_t\|}\rangle + \frac{1}{2}\eta^2(L_0 + L_1\|\nabla\Phi(x_t)\|) \\
&= \Phi(x_t) - \eta\|m_t\| + \eta\langle h_t, \frac{m_t}{\|m_t\|}\rangle + \frac{1}{2}\eta^2(L_0 + L_1\|\nabla\Phi(x_t)\|) \\
&\le \Phi(x_t) - \eta\|m_t\| + \eta\|h_t\| + \frac{1}{2}\eta^2(L_0 + L_1\|\nabla\Phi(x_t)\|) \\
&\le \Phi(x_t) - \eta\|\nabla\Phi(x_t)\| + 2\eta\|h_t\| + \frac{1}{2}\eta^2(L_0 + L_1\|\nabla\Phi(x_t)\|),
\end{aligned} \tag{53}$$

where for the last two lines we use Cauchy-Schwarz inequality and $\|h_t\| = \|\nabla\Phi(x_t) + h_t\| \ge \|\nabla\Phi(x_t)\| - \|h_t\|$. Now expanding h_t by triangle inequality, we have

$$\begin{aligned}
\|h_t\| &= \|m_t - \nabla\Phi(x_t)\| \\
&\le \|m_t - \mathbb{E}_t[\bar{\nabla}f(x_t,\hat{y}_t;\bar{\xi}_t)]\| + \|\mathbb{E}_t[\bar{\nabla}f(x_t,\hat{y}_t;\bar{\xi}_t)] - \bar{\nabla}f(x_t,\hat{y}_t)\| + \|\bar{\nabla}f(x_t,\hat{y}_t) - \nabla\Phi(x_t)\| \\
&\le \|\epsilon_t\| + \frac{l_{g,1}l_{f,0}}{\mu}\left(1-\frac{\mu}{l_{g,1}}\right)^Q + (L_0 + L_1\|\nabla\Phi(x_t)\|)\|\hat{y}_t - y_t^*\|,
\end{aligned}$$

where we use definition of ϵ_t, Lemmas B.4 and B.5 in the last inequality. Plugging the above inequality back into (53) we obtain

$$\begin{aligned}
\Phi(x_{t+1}) &\le \Phi(x_t) - \eta\|\nabla\Phi(x_t)\| + 2\eta\|\epsilon_t\| + 2\eta\frac{l_{g,1}l_{f,0}}{\mu}\left(1-\frac{\mu}{l_{g,1}}\right)^Q \\
&\quad + 2\eta(L_0 + L_1\|\nabla\Phi(x_t)\|)\|\hat{y}_t - y_t^*\| + \frac{1}{2}\eta^2(L_0 + L_1\|\nabla\Phi(x_t)\|) \\
&= \Phi(x_t) - \left(\eta - \frac{1}{2}\eta^2 L_1 - 2\eta L_1\|\hat{y}_t - y_t^*\|\right)\|\nabla\Phi(x_t)\| + 2\eta\|\epsilon_t\| \\
&\quad + 2\eta\frac{l_{g,1}l_{f,0}}{\mu}\left(1-\frac{\mu}{l_{g,1}}\right)^Q + 2\eta L_0\|\hat{y}_t - y_t^*\| + \frac{1}{2}\eta^2 L_0.
\end{aligned}$$

Dividing $1/T\eta$ on both sides, then taking telescope sum and total expectation, and rearranging it finally yields

$$\left(1-\frac{1}{2}\eta L_1-2L_1\|\hat{y}_t-y_t^*\|\right)\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\nabla\Phi(x_t)\|$$
$$\leq\frac{\Phi(x_0)-\Phi(x_T)}{T\eta}+\frac{2}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\epsilon_t\|+\frac{2l_{g,1}l_{f,0}}{\mu}\left(1-\frac{\mu}{l_{g,1}}\right)^Q+\frac{2L_0}{T}\sum_{t=0}^{T-1}\|\hat{y}_t-y_t^*\|+\frac{1}{2}\eta L_0.$$

□

Theorem E.2 (Restatement of Theorem 4.1)**.** *Suppose Assumptions 3.1 to 3.4 hold. Let $\{x_t\}$ be the iterates produced by Algorithm 2. For any given $\delta\in(0,1)$ and any small $\epsilon>0$ satisfying*

$$\epsilon\leq\min\left\{\frac{L_0}{32L_1},\frac{l_{g,1}L_0}{\mu\bar{L}_1},\frac{L_0}{8\bar{L}_1},\frac{L_0l_{g,1}\tilde{\sigma}_{g,1}}{\mu^2},\frac{L_0}{\mu}\sqrt{\frac{l_{g,1}\tilde{\sigma}_{g,1}}{L_1}},\left(\frac{164\cdot 32ed_0L_0^2\tilde{\sigma}_{g,1}^2}{\delta\mu^2}\max\left\{\frac{l_{g,1}}{\tilde{\sigma}_{g,1}},\frac{\bar{\sigma}}{d_0}\right\}\right)^{1/3}\right\},\tag{54}$$

if $\sigma_{g,1}$ satisfies

$$\sigma_{g,1}=\left(\min\left\{\frac{\mu^2\epsilon^2}{164\cdot 16L_0^2\tilde{\sigma}_{g,1}^2\ln(P)},\frac{l_{g,1}}{4\tilde{\sigma}_{g,1}L_1},\frac{\epsilon^2}{4\bar{\sigma}^2}\right\}\right)^{1/4}\tilde{\sigma}_{g,1}\tag{55}$$

with $\tilde{\sigma}_{g,1}=O(1)$, and we set parameters $\alpha,\alpha^{\text{init}},\beta,\gamma,\eta,\tau,I,N,S,Q,T_0$ as

$$1-\beta=\min\left\{\frac{\mu^2\epsilon^2}{164\cdot 16L_0^2\tilde{\sigma}_{g,1}^2\ln(P)},\frac{l_{g,1}}{4\tilde{\sigma}_{g,1}L_1},\frac{\epsilon^2}{4\bar{\sigma}^2}\right\},\quad\eta=\min\left\{\frac{\tilde{\sigma}_{g,1}}{l_{g,1}},\frac{d_0}{\bar{\sigma}}\right\}(1-\beta),\tag{56}$$

$$\alpha^{\text{init}}=\frac{1-\beta}{\mu+l_{g,1}}\quad\alpha=\frac{1-\beta}{\mu},\quad\gamma=\frac{1-\sqrt{\mu\alpha}}{1+\sqrt{\mu\alpha}},\quad\tau=1-\sqrt{\mu\alpha},\tag{57}$$

$$T_0=\ln\left(\frac{\mu^3\alpha^3\epsilon^2}{256L_0^2\|y_0^{\text{init}}-y_0^*\|^2}\right)\Big/\ln\left(1-\frac{\mu\alpha}{4}\right),\tag{58}$$

$$I=\frac{\mu\epsilon}{2(1-\beta)L_0\tilde{\sigma}_{g,1}},\quad N=\ln\left(\frac{\mu\alpha}{128}\right)\Big/\ln\left(1-\frac{\sqrt{\mu\alpha}}{4}\right),\tag{59}$$

$$S=\max\left\{128\ln(P),\frac{128\bar{L}_0^2}{L_0^2}\ln(P),\frac{\mu^2\bar{L}_0^2}{l_{g,1}^2L_0^2}\right\},\quad Q=\ln\left(1-\frac{\mu}{l_{g,1}}\right)\Big/\ln\left(\frac{\mu\epsilon}{l_{g,1}l_{f,0}}\right),\tag{60}$$

where d_0 and P are defined in (37)*. Then with probability at least $1-2\delta$ over the randomness in $\sigma(\mathcal{F}^{\text{init}}\cup\widetilde{\mathcal{F}}_T^1)$ (for Option I) or $\sigma(\mathcal{F}^{\text{init}}\cup(\cup_{t\leq T}\widetilde{\mathcal{F}}_t^2))$ (for Option II), Algorithm 2 guarantees $\frac{1}{T}\sum_{t=1}^T\mathbb{E}\|\nabla\Phi(x_t)\|\leq 20\epsilon$ within $T=\frac{4d_0}{\eta\epsilon}=\widetilde{O}(1/\epsilon^3)$ iterations, where the expectation is taken over the randomness in $\mathcal{F}_T$. For Option I, it requires $T_0+SQT=\widetilde{O}(1/\epsilon^3)$ oracle calls of stochastic gradient or Hessian/Jacobian vector product. For Option II, it requires $T_0+\frac{NT}{I}+SQT=\widetilde{O}(1/\epsilon^3)$ oracle calls of stochastic gradient or Hessian/Jacobian vector product.*

Proof of Theorem E.2. By Lemmas D.6 and E.1, we have

$$\left(1-\frac{1}{2}\eta L_1-2L_1\|\hat{y}_t-y_t^*\|\right)\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\nabla\Phi(x_t)\|$$
$$\leq\frac{\Phi(x_0)-\Phi(x_T)}{T\eta}+\frac{2}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\epsilon_t\|+\frac{2l_{g,1}l_{f,0}}{\mu}\left(1-\frac{\mu}{l_{g,1}}\right)^Q+\frac{2L_0}{T}\sum_{t=0}^{T-1}\|\hat{y}_t-y_t^*\|+\frac{1}{2}\eta L_0$$
$$\leq\frac{d_0}{T\eta}+\frac{2l_{g,1}l_{f,0}}{\mu}\left(1-\frac{\mu}{l_{g,1}}\right)^Q+\frac{2L_0}{T}\sum_{t=0}^{T-1}\|\hat{y}_t-y_t^*\|+\frac{1}{2}\eta L_0$$
$$+\frac{2\bar{\sigma}}{T(1-\beta)}+2\sqrt{1-\beta}\bar{\sigma}+\frac{2\bar{L}_0}{\sqrt{1-\beta}}\sqrt{\frac{2(\eta^2+\vartheta^2)}{S}}+2\bar{L}_1\sqrt{\frac{2(\eta^2+\vartheta^2)}{S(1-\beta)}}\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\nabla\Phi(x_t)\|.$$

Rearranging the above inequality gives

$$\underbrace{\left(1-\frac{1}{2}\eta L_1 - 2L_1\|\hat{y}_t - y_t^*\| - 2\bar{L}_1\sqrt{\frac{2(\eta^2+\vartheta^2)}{S(1-\beta)}}\right)}_{\text{(LHS)}}\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\nabla\Phi(x_t)\|$$

$$\leq \underbrace{\frac{d_0}{T\eta} + \frac{2l_{g,1}l_{f,0}}{\mu}\left(1-\frac{\mu}{l_{g,1}}\right)^Q + \frac{2L_0}{T}\sum_{t=0}^{T-1}\|\hat{y}_t - y_t^*\| + \frac{1}{2}\eta L_0 + \frac{2\bar{\sigma}}{T(1-\beta)} + 2\sqrt{1-\beta}\bar{\sigma} + \frac{2\bar{L}_0}{\sqrt{1-\beta}}\sqrt{\frac{2(\eta^2+\vartheta^2)}{S}}}_{\text{(RHS)}}.$$

Bounding (LHS). By Lemma D.5, we have

$$\begin{aligned}\text{(LHS)} &\geq 1 - \frac{\tilde{\sigma}_{g,1}L_1}{2l_{g,1}}(1-\beta) - 2L_1\frac{2\epsilon}{L_0} - 2\bar{L}_1\sqrt{\frac{2(\eta^2+\vartheta^2)}{S(1-\beta)}} \\ &\geq 1 - \frac{1}{8} - \frac{1}{8} - \frac{1}{4} = \frac{1}{2}\end{aligned} \tag{61}$$

Bounding (RHS). By choice of parameters, we have

$$\text{(RHS)} \leq \frac{1}{4}\epsilon + 2\epsilon + 4\epsilon + \epsilon + \frac{1}{2}\epsilon + \epsilon + \epsilon \leq 10\epsilon. \tag{62}$$

Combining (61) and (62) finally yields

$$\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\|\nabla\Phi(x_t)\| \leq 20\epsilon.$$

□

F Omitted Proofs in Appendix B

F.1 Proof of Lemma B.5

Lemma F.1 (Restatement of Lemma B.5)**.** *Under Assumptions 3.1 to 3.4, we have*

$$\|\bar{\nabla}f(x,y) - \nabla\Phi(x)\| \leq (\bar{L} + L_{x,1}\|\nabla\Phi(x)\|)\|y - y^*(x)\|,$$

where constant $\bar{L}$ is defined as

$$\bar{L} \coloneqq L_{x,0} + L_{x,1}\frac{l_{g,1}l_{f,0}}{\mu} + \frac{l_{g,1}}{\mu}(L_{y,0} + L_{y,1}l_{f,0}) + l_{f,0}\frac{\mu l_{g,2} + l_{g,1}l_{g,2}}{\mu^2} \leq L_0.$$

Proof of Lemma B.5. Recall that the exact expressions of $\bar{\nabla}f(x,y)$ and $\nabla\Phi(x)$ are

$$\bar{\nabla}f(x,y) = \nabla_x f(x,y) - \nabla_{xy}^2 g(x,y)[\nabla_{yy}^2 g(x,y)]^{-1}\nabla_y f(x,y)$$

and

$$\nabla\Phi(x) = \nabla_x f(x,y^*(x)) - \nabla_{xy}^2 g(x,y^*(x))[\nabla_{yy}^2 g(x,y^*(x))]^{-1}\nabla_y f(x,y^*(x)).$$

Then by Assumption 3.2 we have

$$\begin{aligned}&\|\bar{\nabla}f(x,y) - \nabla\Phi(x)\| \leq \|\nabla_x f(x,y) - \nabla_x f(x,y^*(x))\| \\ &\quad + \|\nabla_{xy}^2 g(x,y)[\nabla_{yy}^2 g(x,y)]^{-1}\nabla_y f(x,y) - \nabla_{xy}^2 g(x,y^*(x))[\nabla_{yy}^2 g(x,y^*(x))]^{-1}\nabla_y f(x,y^*(x))\| \\ &\leq (L_{x,0} + L_{x,1}\|\nabla_x f(x,y^*(x))\|)\|y - y^*(x)\| \\ &\quad + \|\nabla_{xy}^2 g(x,y)[\nabla_{yy}^2 g(x,y)]^{-1}\nabla_y f(x,y) - \nabla_{xy}^2 g(x,y^*(x))[\nabla_{yy}^2 g(x,y)]^{-1}\nabla_y f(x,y)\| \\ &\quad + \|\nabla_{xy}^2 g(x,y^*(x))[\nabla_{yy}^2 g(x,y)]^{-1}\nabla_y f(x,y) - \nabla_{xy}^2 g(x,y^*(x))[\nabla_{yy}^2 g(x,y^*(x))]^{-1}\nabla_y f(x,y)\| \\ &\quad + \|\nabla_{xy}^2 g(x,y^*(x))[\nabla_{yy}^2 g(x,y^*(x))]^{-1}\nabla_y f(x,y) - \nabla_{xy}^2 g(x,y^*(x))[\nabla_{yy}^2 g(x,y^*(x))]^{-1}\nabla_y f(x,y^*(x))\|\end{aligned}$$

$$
\begin{aligned}
&\leq \left(L_{x,0} + L_{x,1}\left(\frac{l_{g,1}l_{f,0}}{\mu} + \|\nabla\Phi(x)\|\right)\right)\|y - y^*(x)\| \\
&\quad + \frac{l_{f,0}}{\mu}l_{g,2}\|y - y^*(x)\| + \frac{l_{f,0}l_{g,1}}{\mu^2}l_{g,2}\|y - y^*(x)\| + \frac{l_{g,1}}{\mu}(L_{y,0} + L_{y,1}\|\nabla_y f(x, y^*(x))\|)\|y - y^*(x)\| \\
&= \left(L_{x,0} + L_{x,1}\frac{l_{g,1}l_{f,0}}{\mu} + \frac{l_{g,1}}{\mu}(L_{y,0} + L_{y,1}l_{f,0}) + l_{f,0}\frac{\mu l_{g,2} + l_{g,1}l_{g,2}}{\mu^2} + L_{x,1}\|\nabla\Phi(x)\|\right)\|y - y^*(x)\|.
\end{aligned}
$$

By definition of $\bar{L}$ we conclude the proof. □

F.2 Proof of Lemma B.6

Lemma F.2 (Restatement of Lemma B.6)**.** *Under Assumptions 3.1 to 3.4, we have*

(i) For any fixed $y \in \mathbb{R}^{d_y}$ and any $x_1, x_2 \in \mathbb{R}^{d_x}$,

$$\mathbb{E}_{\bar{\xi}}\|\bar{\nabla} f(x_1, y; \bar{\xi}) - \bar{\nabla} f(x_2, y; \bar{\xi})\|^2 \leq (\bar{L}_0^2 + \bar{L}_1^2\|\nabla\Phi(x_1)\|^2)\|x_1 - x_2\|^2.$$

(ii) For any fixed $x \in \mathbb{R}^{d_x}$ and any $y_1, y_2 \in \mathbb{R}^{d_y}$,

$$\mathbb{E}_{\bar{\xi}}\|\bar{\nabla} f(x, y_1; \bar{\xi}) - \bar{\nabla} f(x, y_2; \bar{\xi})\|^2 \leq (\bar{L}_0^2 + \bar{L}_1^2\|\nabla\Phi(x_1)\|^2)\|x_1 - x_2\|^2.$$

In the above expressions, we define $\bar{L}_0$ and $\bar{L}_1$ as

$$
\begin{aligned}
\bar{L}_0 = \Bigg\{ & 4\left(L_{x,0} + L_{x,1}\left(\frac{l_{g,1}l_{f,0}}{\mu} + \left(L_{x,0} + \frac{L_{x,1}l_{g,1}l_{f,0}}{\mu}\right)\|y_1 - y_1^*\|\right)\right)^2 \\
& + \frac{6Q}{2\mu l_{g,1} - \mu^2}\left(l_{g,1}^2(L_{y,0} + L_{y,1}l_{f,0})^2 + l_{f,0}^2 l_{g,2}^2 + \frac{l_{f,0}^2 l_{g,1}^2 l_{g,2}^2 K^2}{(l_{g,1} - \mu)^2}\right)\Bigg\}^{1/2}, \\
\bar{L}_1 = 2L_{x,1}(1 + L_{x,1}\|y_1 - y_1^*\|).
\end{aligned}
$$

Proof of Lemma B.6. We show statement (i) of the lemma, and (ii) follows by similar arguments. For any fixed $y \in \mathbb{R}^{d_y}$ and any $x_1, x_2 \in \mathbb{R}^{d_x}$, by definition of $\bar{\nabla} f(x, y; \bar{\xi})$ we have

$$
\begin{aligned}
&\|\bar{\nabla} f(x_1, y; \bar{\xi}) - \bar{\nabla} f(x_2, y; \bar{\xi})\|^2 \\
&\leq 2\|\nabla_x F(x_1, y; \xi) - \nabla_x F(x_2, y; \xi)\|^2 + 2\Bigg\|\nabla_{xy}^2 G(x_1, y; \zeta^{(0)})\left[\frac{Q}{l_{g,1}}\prod_{i=1}^{\mathsf{q}}\left(I - \frac{1}{l_{g,1}}\nabla_{yy}^2 G(x_1, y; \zeta^{(i)})\right)\right]\nabla_y F(x_1, y; \xi) \\
&\qquad - \nabla_{xy}^2 G(x_2, y; \zeta^{(0)})\left[\frac{Q}{l_{g,1}}\prod_{i=1}^{\mathsf{q}}\left(I - \frac{1}{l_{g,1}}\nabla_{yy}^2 G(x_2, y; \zeta^{(i)})\right)\right]\nabla_y F(x_2, y; \xi)\Bigg\|^2 \\
&\leq 2(L_{x,0} + L_{x,1}\|\nabla_x f(x_1, y)\|)^2\|x_1 - x_2\|^2 + 2\Bigg\|\nabla_{xy}^2 G(x_1, y; \zeta^{(0)})\left[\frac{Q}{l_{g,1}}\prod_{i=1}^{\mathsf{q}}\left(I - \frac{1}{l_{g,1}}\nabla_{yy}^2 G(x_1, y; \zeta^{(i)})\right)\right]\nabla_y F(x_1, y; \xi) \\
&\qquad - \nabla_{xy}^2 G(x_2, y; \zeta^{(0)})\left[\frac{Q}{l_{g,1}}\prod_{i=1}^{\mathsf{q}}\left(I - \frac{1}{l_{g,1}}\nabla_{yy}^2 G(x_2, y; \zeta^{(i)})\right)\right]\nabla_y F(x_2, y; \xi)\Bigg\|^2.
\end{aligned}
$$

For the second term above, we have

$$
\begin{aligned}
&\Bigg\|\nabla_{xy}^2 G(x_1, y; \zeta^{(0)})\left[\frac{Q}{l_{g,1}}\prod_{i=1}^{\mathsf{q}}\left(I - \frac{1}{l_{g,1}}\nabla_{yy}^2 G(x_1, y; \zeta^{(i)})\right)\right]\nabla_y F(x_1, y; \xi) \\
&\qquad - \nabla_{xy}^2 G(x_2, y; \zeta^{(0)})\left[\frac{Q}{l_{g,1}}\prod_{i=1}^{\mathsf{q}}\left(I - \frac{1}{l_{g,1}}\nabla_{yy}^2 G(x_2, y; \zeta^{(i)})\right)\right]\nabla_y F(x_2, y; \xi)\Bigg\|^2 \\
&\leq 3l_{g,1}^2\frac{Q^2}{l_{g,1}^2}\left(1 - \frac{\mu}{l_{g,1}}\right)^{2\mathsf{q}}\|\nabla_y F(x_1, y; \xi) - \nabla_y F(x_2, y; \xi)\|^2 \\
&\qquad + 3l_{f,0}^2\frac{Q^2}{l_{g,1}^2}\left(1 - \frac{\mu}{l_{g,1}}\right)^{2\mathsf{q}}\|\nabla_{xy}^2 G(x_1, y; \zeta^{(0)}) - \nabla_{xy}^2 G(x_2, y; \zeta^{(0)})\|^2
\end{aligned}
$$

$$
\begin{aligned}
&+ 3l_{g,1}^2 l_{f,0}^2 \left\| \frac{Q}{l_{g,1}} \prod_{i=1}^{\mathsf{q}} \left(I - \frac{1}{l_{g,1}} \nabla_{yy}^2 G(x_1, y; \zeta^{(i)}) \right) - \frac{Q}{l_{g,1}} \prod_{i=1}^{\mathsf{q}} \left(I - \frac{1}{l_{g,1}} \nabla_{yy}^2 G(x_2, y; \zeta^{(i)}) \right) \right\|^2 \\
\leq\ & 3Q^2 \left(1 - \frac{\mu}{l_{g,1}}\right)^{2\mathsf{q}} (L_{y,0} + L_{y,1} \|\nabla_y f(x_1, y)\|)^2 \|x_1 - x_2\|^2 + 3 \frac{l_{f,0}^2 Q^2}{l_{g,1}^2} \left(1 - \frac{\mu}{l_{g,1}}\right)^{2\mathsf{q}} l_{g,2}^2 \|x_1 - x_2\|^2 \\
&+ 3l_{f,0}^2 Q^2 \left\| \prod_{i=1}^{\mathsf{q}} \left(I - \frac{1}{l_{g,1}} \nabla_{yy}^2 G(x_1, y; \zeta^{(i)}) \right) - \prod_{i=1}^{\mathsf{q}} \left(I - \frac{1}{l_{g,1}} \nabla_{yy}^2 G(x_2, y; \zeta^{(i)}) \right) \right\|^2 .
\end{aligned}
$$

Then we take expectation with respect to q and obtain

$$
\begin{aligned}
&\mathbb{E}_{\mathsf{q}} \left\| \nabla_{xy}^2 G(x_1, y; \zeta^{(0)}) \left[\frac{Q}{l_{g,1}} \prod_{i=1}^{\mathsf{q}} \left(I - \frac{1}{l_{g,1}} \nabla_{yy}^2 G(x_1, y; \zeta^{(i)}) \right) \right] \nabla_y F(x_1, y; \xi) \right. \\
&\qquad \left. - \nabla_{xy}^2 G(x_2, y; \zeta^{(0)}) \left[\frac{Q}{l_{g,1}} \prod_{i=1}^{\mathsf{q}} \left(I - \frac{1}{l_{g,1}} \nabla_{yy}^2 G(x_2, y; \zeta^{(i)}) \right) \right] \nabla_y F(x_2, y; \xi) \right\|^2 \\
\leq\ & \left(3Q^2 (L_{y,0} + L_{y,1} \|\nabla_y f(x_1, y)\|)^2 \|x_1 - x_2\|^2 + 3 \frac{l_{f,0}^2 Q^2}{l_{g,1}^2} l_{g,2}^2 \|x_1 - x_2\|^2 \right) \mathbb{E}_{\mathsf{q}} \left[\left(1 - \frac{\mu}{l_{g,1}}\right)^{2\mathsf{q}} \right] \\
&+ 3l_{f,0}^2 Q^2 \mathbb{E}_{\mathsf{q}} \left\| \prod_{i=1}^{\mathsf{q}} \left(I - \frac{1}{l_{g,1}} \nabla_{yy}^2 G(x_1, y; \zeta^{(i)}) \right) - \prod_{i=1}^{\mathsf{q}} \left(I - \frac{1}{l_{g,1}} \nabla_{yy}^2 G(x_2, y; \zeta^{(i)}) \right) \right\|^2 \\
\leq\ & \left(3Q^2 (L_{y,0} + L_{y,1} \|\nabla_y f(x_1, y)\|)^2 \|x_1 - x_2\|^2 + 3 \frac{l_{f,0}^2 Q^2}{l_{g,1}^2} l_{g,2}^2 \|x_1 - x_2\|^2 \right) \cdot \frac{l_{g,1}^2}{Q(2\mu l_{g,1} - \mu^2)} \\
&+ 3l_{f,0}^2 Q^2 \cdot \frac{l_{g,1}^2 l_{g,2}^2 Q}{(l_{g,1} - \mu)^2 (2\mu l_{g,1} - \mu^2)} \|x_1 - x_2\|^2 \\
\leq\ & \frac{3Q}{2\mu l_{g,1} - \mu^2} \left(l_{g,1}^2 (L_{y,0} + L_{y,1} l_{f,0})^2 \|x_1 - x_2\|^2 + l_{f,0}^2 l_{g,2}^2 \|x_1 - x_2\|^2 \right) + \frac{3l_{f,0}^2 l_{g,1}^2 l_{g,2}^2 Q^3}{(l_{g,1} - \mu)^2 (2\mu l_{g,1} - \mu^2)} \|x_1 - x_2\|^2 \\
=\ & \frac{3Q}{2\mu l_{g,1} - \mu^2} \left(l_{g,1}^2 (L_{y,0} + L_{y,1} l_{f,0})^2 + l_{f,0}^2 l_{g,2}^2 + \frac{l_{f,0}^2 l_{g,1}^2 l_{g,2}^2 Q^2}{(l_{g,1} - \mu)^2} \right) \|x_1 - x_2\|^2
\end{aligned}
$$

Finally, taking expectation on both sides yields

$$
\begin{aligned}
\mathbb{E}_{\bar{\xi}} \|\bar{\nabla} f(x_1, y; \bar{\xi}) - \bar{\nabla} f(x_2, y; \bar{\xi})\|^2 \leq\ & 2(L_{x,0} + L_{x,1} \|\nabla_x f(x_1, y)\|)^2 \|x_1 - x_2\|^2 \\
&+ \frac{6Q}{2\mu l_{g,1} - \mu^2} \left(l_{g,1}^2 (L_{y,0} + L_{y,1} l_{f,0})^2 + l_{f,0}^2 l_{g,2}^2 + \frac{l_{f,0}^2 l_{g,1}^2 l_{g,2}^2 Q^2}{(l_{g,1} - \mu)^2} \right) \|x_1 - x_2\|^2 .
\end{aligned}
$$

Since for any $y \in \mathbb{R}^{d_y}$, we have

$$
\begin{aligned}
\|\nabla_x f(x_1, y) - \nabla_x f(x_1, y_1^*)\| &\leq (L_{x,0} + L_{x,1} \|\nabla_x f(x_1, y_1^*)\|) \|y_1 - y_1^*\| \\
&\leq \left(L_{x,0} + L_{x,1} \left(\frac{l_{g,1} l_{f,0}}{\mu} + \|\nabla \Phi(x_1)\| \right) \right) \|y_1 - y_1^*\| \\
&= \left(L_{x,0} + \frac{L_{x,1} l_{g,1} l_{f,0}}{\mu} + L_{x,1} \|\nabla \Phi(x_1)\| \right) \|y_1 - y_1^*\|,
\end{aligned}
$$

which yields

$$
\begin{aligned}
\|\nabla_x f(x_1, y)\| &\leq \|\nabla_x f(x_1, y_1^*)\| + \left(L_{x,0} + \frac{L_{x,1} l_{g,1} l_{f,0}}{\mu} + L_{x,1} \|\nabla \Phi(x_1)\| \right) \|y_1 - y_1^*\| \\
&\leq \frac{l_{g,1} l_{f,0}}{\mu} + \|\nabla \Phi(x_1)\| + \left(L_{x,0} + \frac{L_{x,1} l_{g,1} l_{f,0}}{\mu} + L_{x,1} \|\nabla \Phi(x_1)\| \right) \|y_1 - y_1^*\| \\
&= \left(\frac{l_{g,1} l_{f,0}}{\mu} + \left(L_{x,0} + \frac{L_{x,1} l_{g,1} l_{f,0}}{\mu} \right) \|y_1 - y_1^*\| \right) + (1 + L_{x,1} \|y_1 - y_1^*\|) \|\nabla \Phi(x_1)\|.
\end{aligned}
$$

Therefore, we conclude that

$$
\begin{aligned}
\mathbb{E}_{\bar{\xi}}\|\bar{\nabla} f(x_1,y;\bar{\xi})-\bar{\nabla} f(x_2,y;\bar{\xi})\|^2 &\leq 2(L_{x,0}+L_{x,1}\|\nabla_x f(x_1,y)\|)^2\|x_1-x_2\|^2 \\
&\quad + \frac{6Q}{2\mu l_{g,1}-\mu^2}\left(l_{g,1}^2(L_{y,0}+L_{y,1}l_{f,0})^2+l_{f,0}^2 l_{g,2}^2+\frac{l_{f,0}^2 l_{g,1}^2 l_{g,2}^2 Q^2}{(l_{g,1}-\mu)^2}\right)\|x_1-x_2\|^2 \\
&\leq 2\left(L_{x,0}+L_{x,1}\left(\frac{l_{g,1}l_{f,0}}{\mu}+\left(L_{x,0}+\frac{L_{x,1}l_{g,1}l_{f,0}}{\mu}\right)\|y_1-y_1^*\|\right)+L_{x,1}(1+L_{x,1}\|y_1-y_1^*\|)\|\nabla\Phi(x_1)\|\right)^2\|x_1-x_2\|^2 \\
&\quad + \frac{6Q}{2\mu l_{g,1}-\mu^2}\left(l_{g,1}^2(L_{y,0}+L_{y,1}l_{f,0})^2+l_{f,0}^2 l_{g,2}^2+\frac{l_{f,0}^2 l_{g,1}^2 l_{g,2}^2 Q^2}{(l_{g,1}-\mu)^2}\right)\|x_1-x_2\|^2 \\
&\leq 4\left(L_{x,0}+L_{x,1}\left(\frac{l_{g,1}l_{f,0}}{\mu}+\left(L_{x,0}+\frac{L_{x,1}l_{g,1}l_{f,0}}{\mu}\right)\|y_1-y_1^*\|\right)\right)^2\|x_1-x_2\|^2 \\
&\quad + 4L_{x,1}^2(1+L_{x,1}\|y_1-y_1^*\|)^2\|\nabla\Phi(x_1)\|^2\|x_1-x_2\|^2 \\
&\quad + \frac{6Q}{2\mu l_{g,1}-\mu^2}\left(l_{g,1}^2(L_{y,0}+L_{y,1}l_{f,0})^2+l_{f,0}^2 l_{g,2}^2+\frac{l_{f,0}^2 l_{g,1}^2 l_{g,2}^2 Q^2}{(l_{g,1}-\mu)^2}\right)\|x_1-x_2\|^2 \\
&= (\bar{L}_0^2+\bar{L}_1^2\|\nabla\Phi(x_1)\|^2)\|x_1-x_2\|^2,
\end{aligned}
$$

where we use the definition of $\bar{L}_0$ and $\bar{L}_1$ in the last equality. □

G Additional Experimental Details

Hyerparameter setting. We tune the best hyperparameters for each algorithm, including upper-/lower-level step size, the number of inner loops, momentum parameters, etc. The upper-level learning rate η_{up} and lower-level learing rate η_{low} are tuned in the range of $[0.001, 0.1]$ for all the baselines on experiments of AUC maximization and data hyper-cleaning, the best (η_{up}, η_{low}) on **AUC maximization** are summarized as follows: StocBio: $(0.01, 0.001)$, TTSA: $(0.005, 0.01)$, SABA: $(0.01, 0.005)$, MA-SOBA: $(0.01, 0.005)$, SUSTAIN: $(0.03, 0.01)$, VRBO: $(0.05, 0.01)$, BO-REP: $(0.001, 0.001)$, AccBO: $(0.005, 0.005)$. The best learning rate on the experiment of **data hyper-cleaning** are summarized as follows: Stocbio: $(0.01, 0.002)$, TTSA: $(0.001, 0.01)$, SABA: $(0.05, 0.02)$, MA-SOBA: $(0.01, 0.01)$, SUSTAIN: $(0.05, 0.05)$, VRBO: $(0.1, 0.05)$, BO-REP: $(0.02, 0.01)$, AccBO: $(0.1, 0.1)$. Note that SUSTAIN decays its upper-/lower-level step size with epoch (t) by $\eta_{up} = \eta_{up}/(t+2)^{1/3}$, $\eta_{low} = \eta_{up}/(t+2)^{1/3}$, while other algorithms use a constant learning rate. The number for neumann series estimation in StocBiO and VRBO is fixed to 3, while it is uniformly sampled from $\{1, 2, 3\}$ in TTSA, SUSTAIN, and AccBO. In AUC maximization, AccBO uses Option I (Option II in data hyper-cleaning) to update the lower-level variable, and sets the Nestrov momentum parameter $\gamma = 0.5$, the averaging parameter $\tau = 0.5$ ($\gamma = 0.1$ and $\tau = 0.5$ in data hyper-cleaning). In AUC maximization, the batch size is set to be 32 for all algorithms except VRBO, which uses larger batch size of 64 (tuned in the range of $\{32, 64, 128, 256, 512\}$) at the checkpoint step and 32 otherwise. In data hyper-cleaning, the batch size is set to be 128 for all algorithms except VRBO, which uses larger batch size of 256 (tuned in the range of $\{63, 128, 256, 512, 1024\}$) at the checkpoint step and 128 otherwise. AccBO uses Option II in data hyper-cleaning, and the periodical update for low-level variable sets the iterations $N = 3$ and update interval $I = 2$. Other hyperparameters setting keep the same in AUC maximization and data hyper-cleaning: The momentum parameter β is fixed to 0.9 in AccBO, MA-SOBA, BO-REP. The warm start steps for lower-level variable in AccBO is set to 3. The number of inner loops for StocBio is set to 3. BO-REP uses the periodical update for low-level variable, and set the iterations $N = 3$ and the update interval $I = 2$.

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