Accelerating Inexact HyperGradient Descent for Bilevel Optimization

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Abstract

We present a method for solving general nonconvex-strongly-convex bilevel optimization problems. Our method—the *Restarted Accelerated HyperGradient Descent* (`RAHGD`) method—finds an ϵ-first-order stationary point of the objective with $\tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$ oracle complexity, where κ is the condition number of the lower-level objective and ϵ is the desired accuracy. We also propose a perturbed variant of `RAHGD` for finding an $\big(\epsilon, \mathcal{O}(\kappa^{2.5}\sqrt{\epsilon}\,)\big)$-second-order stationary point within the same order of oracle complexity. Our results achieve the best-known theoretical guarantees for finding stationary points in bilevel optimization and also improve upon the existing upper complexity bound for finding second-order stationary points in nonconvex-strongly-concave minimax optimization problems, setting a new state-of-the-art benchmark. Empirical studies are conducted to validate the theoretical results in this paper.

1 Introduction

Bilevel optimization is emerging as a key unifying problem formulation in machine learning, encompassing a variety of applications including meta-learning, model-free reinforcement learning and hyperparameter optimization (Franceschi et al., 2018; Stadie et al., 2020). Our work focuses on a version of the general problem that is particularly relevant to machine learning—the *nonconvex-strongly-convex bilevel optimization problem*:

$$\min_{x\in\mathbb{R}^{d_x}} \ \Phi(x) \triangleq f(x, y^*(x)), \tag{1a}$$

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

where the upper-level function $f(x, y)$ is smooth and possibly nonconvex, and the lower-level function $g(x, y)$ is smooth and strongly convex with respect to y for any given x.[1] Bilevel optimization is more expressive but harder to solve than classical single-level optimization, since the objective $\Phi(x)$ in (1a) involves the argument input $y^*(x)$ which is the solution of the lower-level problem (1b). In contrast to classical optimization, the bilevel optimization problem is an optimization problem where the minimization variable is taken as the minimizer of a lower-level optimization problem.

Most existing work on nonconvex-strongly-convex bilevel optimization (Ghadimi & Wang, 2018; Ji et al., 2021, 2022; Kwon et al., 2023) focuses on finding approximate *first-order stationary points* (FOSP) of the objective. Recently, Huang et al. (2022) extended the scope of work in this area, proposing the (perturbed) *approximate implicit differentiation* (AID) algorithm which can find an $\big(\epsilon, \mathcal{O}(\kappa^{2.5}\sqrt{\epsilon}\,)\big)$-*second-order stationary points* (SOSP) within a $\tilde{\mathcal{O}}(\kappa^4\epsilon^{-2})$ oracle complexity, where $\kappa \geq 1$ is the condition number of any $f(x, \cdot)$ and $\epsilon > 0$ is the desired accuracy. Given this result, a key further challenge is to study whether the ϵ^{-2}-dependency in the upper complexity bound can be improved under additional Lipschitz assumptions on high-order derivatives (Huang et al., 2022).[2]

In this context, a natural question to ask is: *Can we design an algorithm that improves upon known algorithmic complexities for finding approximate first-order and second-order stationary points in nonconvex-strongly-convex bilevel optimization?*

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[1] As the reader will see in Lemma 2.6 additional smoothness conditions capture the smoothness of the overall objective function $\Phi(x)$.

[2] It is worth noting that the $O(\epsilon^{-2})$ complexity is *optimal* for finding an *ϵ-first-order stationary point* in terms of the dependency on ϵ under the Lipschitz gradient assumption (Carmon et al., 2020) when κ is treated as an $O(1)$-constant. This is primarily due to the fact that nonconvex optimization can be viewed as a special case of our bilevel problem, and hence the hard instance can be inherited to prove the analogous lower bound.

1.1 Contributions

We resolve this question by designing a particular form of acceleration of hypergradient descent and thereby improving the oracle complexity. Our contributions are four-fold:

(i) We propose a method that we refer to as *Restarted Accelerated Hypergradient Descent* (`RAHGD`) that applies Nesterov's *accelerated gradient descent* (AGD) to approximate the solution $y^*(x)$ of the inner problem (1b) and combines it with the *conjugate gradient* (CG) method to construct an inexact hypergradient of the objective. The algorithm makes use of proper restarting and acceleration to optimize the objective $\Phi(\cdot)$ based on the obtained inexact hypergradient. We show that `RAHGD` can find an ϵ-FOSP of the objective within $\mathcal{O}(\kappa^{3.25}\epsilon^{-1.75})$ first-order oracle queries [Section 3].

(ii) For the task of finding approximate second-order stationary points (SOSPs), we add a perturbation step to `RAHGD` and introduce the *Perturbed Restarted Accelerated HyperGradient Descent* (`PRAHGD`) algorithm. We show that `PRAHGD` can efficiently escape saddle points and find an $\big(\epsilon, \mathcal{O}(\kappa^{2.5}\sqrt{\epsilon}\,)\big)$-second-order stationary point of the objective Φ within $\tilde{\mathcal{O}}\big(\kappa^{3.25}\epsilon^{-1.75}\big)$ first-order oracle queries (including gradient queries and also Jacobian/Hessian-vector-product queries). This improves over the best known complexity in bilevel optimization due to Huang et al. (2022) by a factor of $\tilde{\mathcal{O}}(\kappa^{0.75}\epsilon^{-0.25})$ [Section 4].

(iii) We apply the theoretical framework of `PRAHGD` to the problem of minimax optimization. In particular, we propose a `PRAHGD` variant crafted for nonconvex-strongly-concave minimax optimization. We refer to the resulting algorithm as *Perturbed Restarted Accelerate Gradient Descent Ascent* (`PRAGDA`). We show that `PRAGDA` provably finds an $\mathcal{O}\big(\epsilon, \mathcal{O}(\kappa^{1.5}\sqrt{\epsilon}\,)\big)$-SOSP with a first-order oracle query complexity of $\tilde{\mathcal{O}}(\kappa^{1.75}\epsilon^{-1.75})$. This improves upon the best known first-order (including gradient/Hessian-vector/Jacobian-vector-product) oracle query complexity bound of $\tilde{\mathcal{O}}(\kappa^{1.5}\epsilon^{-2} + \kappa^{2}\epsilon^{-1.5})$ due to Luo et al. (2022) [Section 5].

(iv) We conduct a variety of empirical studies of bilevel optimization. Specifically, we evaluate the effectiveness of our proposed algorithms (`RAHGD` / `PRAHGD` / `PRAGDA`) by applying them to three different tasks: a synthetic minimax problem, data hypercleaning for the MNIST dataset, and hyperparameter optimization for logistic regression. Our studies demonstrate that our algorithms outperform several established baseline algorithms, such as BA (Ghadimi & Wang, 2018), AID-BiO (Ji et al., 2021), ITD-BiO (Ji et al., 2021), Perturbed AID-BiO (Huang et al., 2022) and iMCN (Luo et al., 2022). Overall, the results provide clear evidence in support of the effectiveness of our proposed algorithmic framework for bilevel and minimax optimization [Appendix F].

1.2 Overview of Our Algorithm Design and Main Techniques

We overview the algorithm design in this subsection. Inspired by the success of the accelerated gradient descent method for nonconvex optimization (see, e.g., Carmon et al., 2018; Agarwal et al., 2017; Carmon et al., 2017; Jin et al., 2018; Li & Lin, 2022), we propose a novel method called the *restarted accelerated hypergradient descent* (`RAHGD`) algorithm. The gradient of $\Phi(x)$, which we call the *hypergradient*, can be computed via the following equation (Ghadimi & Wang, 2018; Ji et al., 2021):

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

Unfortunately, directly applying first-order algorithms by iterating with the exact hypergradient $\nabla\Phi(x)$ is costly or intractable for large-scale problems, given the need to obtain $y^*(x)$ and particularly the need to invert the matrix $\nabla^2_{yy} g(x, y^*(x))$.

For given $x = x_k \in \mathbb{R}^{d_x}$, we aim to construct an estimate of $\nabla\Phi(x_k)$ with reasonable computational cost and sufficient accuracy. The strong convexity of $g(x_k, \cdot)$ motivates us to apply AGD for finding $y_k \approx y^*(x_k)$ and hence used as a replacement in estimates of $\nabla\Phi(x_k)$. To avoid direct computation of the term $\big(\nabla^2_{yy} g(x_k, y_k)\big)^{-1}\nabla_y f(x_k, y_k)$, we observe that it is the solution of the following quadratic problem:

$$\min_{v\in\mathbb{R}^{d_y}} \ \frac{1}{2} v^\top \nabla^2_{yy} g(x_k, y_k) v - v^\top \nabla_y f(x_k, y_k). \tag{3}$$

Accordingly, we can efficiently estimate $v_k \approx \big(\nabla^2_{yy} g(x_k, y_k)\big)^{-1}\nabla_y f(x_k, y_k)$ by solving (3) using a conjugate gradient subroutine. Based on y_k and v_k, we obtain the following expression for an *inexact hypergradient*:

$$\hat{\nabla}\Phi(x_k) = \nabla_x f(x_k, y_k) - \nabla^2_{xy} g(x_k, y_k) v_k \tag{4}$$

which can serve as a surrogate of the true hypergradient $\nabla\Phi(x_k)$ in our first-order algorithmic design.

We formally present `RAHGD` in Algorithm 3. The main issue to address for `RAHGD` is the computational cost for achieving sufficient accuracy of $\hat{\nabla}\Phi(x_k)$. Interestingly, our theoretical analysis shows that all of the additional cost arises from the computations of y_k and

v_k, and it can thus be bounded tightly. As a result, our algorithm can find approximate first-order stationary points with smaller oracle complexities than is the case with existing methods (Ghadimi & Wang, 2018; Ji et al., 2021). We also introduce the *perturbed* RAHGD (PRAHGD) in Algorithm 3 for escaping saddle points. Extending the analysis of RAHGD, we show that PRAHGD can find approximate second-order stationary points more efficiently than existing work (Huang et al., 2022).

1.3 Related Work

The subject of bilevel optimization problem has a long history with early work tracing back to the 1970s (Bracken & McGill, 1973). Recent algorithmic advances in this field have had applications in areas such as meta-learning (Bertinetto et al., 2019; Franceschi et al., 2018; Ji et al., 2020), reinforcement learning (Konda & Tsitsiklis, 1999; Stadie et al., 2020; Hong et al., 2023) and hyperparameter optimization (Feurer & Hutter, 2019; Shaban et al., 2019; Grazzi et al., 2020).

There have also been theoretical advances in bilevel optimization in recent years. Ghadimi & Wang (2018) presented a convergence rate for the AID approach when $f(x, y)$ is convex, analyzing the complexity of an accelerated algorithm that uses gradient descent to approximate $y^*(x_k)$ in the inner loop and uses AGD in the outer loop. Further improvements in dependence on the condition number and analysis of the convergence were achieved via the *iterative differentiation* (ITD) approach of Ji et al. (2021, 2022), who analyzed the complexity of AID and ITD and also provided a complexity analysis for a randomized version. Hong et al. (2023) proposed the TTSA algorithm—a single-loop algorithm that updates two variables in an alternating manner—and presented applications to the problem of reinforcement learning under randomized scenarios. For stochastic bilevel problems, various methods have been proposed, such as BSA Ghadimi & Wang (2018), TTSA Hong et al. (2023), stocBiO Ji et al. (2021), and ALSET Chen et al. (2021a). More recent research on this front has focused on variance reduction and momentum techniques, resulting in cutting-edge stochastic oracle complexities (Ji & Liang, 2023; Li et al., 2022; Kwon et al., 2023).

While much of the literature on bilevel optimization has focused on finding first-order stationary points, the problem of finding second-order stationary points has been largely unaddressed. Huang et al. (2022) recently proposed a perturbed algorithm for finding approximate second-order stationary points. The algorithm adopts gradient descent (GD) to approximately solve the lower-level minimization problem and conjugate gradient (CG) to solve for Hessian-vector product with GD used in the outer loop. For the problem of classical optimization, second-order methods such as those proposed in Nesterov & Polyak (2006); Curtis et al. (2017) have been used to obtain ϵ-accurate SOSPs in single-level optimization with a complexity of $\mathcal{O}(\epsilon^{-1.5})$; however, they require expensive operations such as estimating the inverse of Hessian matrices. A significant body of recent literature has focuses on first-order methods for obtaining an approximate $\big(\epsilon, \mathcal{O}(\kappa^{2.5}\sqrt{\epsilon})\big)$-SOSP, with a best-known complexity of $\tilde{\mathcal{O}}(\epsilon^{-1.75})$ in terms of gradient and Hessian-vector products (Agarwal et al., 2017; Carmon et al., 2018, 2017; Jin et al., 2017, 2018; Li & Lin, 2022).

An important special case of the bilevel optimization problem (1)—the problem of minimax optimization, where $g = -f$ in Eq. (1b)—has been extensively studied in the literature. Minimax optimization has been the focus of attention in the machine learning community recently due to its applications to training GANs (Goodfellow et al., 2020; Arjovsky et al., 2017), to adversarial learning (Goodfellow et al., 2015; Sinha et al., 2018) and to optimal transport (Lin et al., 2020a; Huang et al., 2021). On the theoretical front, Nouiehed et al. (2019); Jin et al. (2020) studied the complexity of Multistep Gradient Descent Ascent (GDmax), and Lin et al. (2020b); Lu et al. (2020) provided the first convergence analysis for the single-loop *gradient descent ascent* (GDA) algorithm for finding first-order stationary point. Luo et al. (2020) applied the stochastic variance reduction technique to the nonconvex-strongly-concave case, achieving the first optimal complexity upper bound in stochastic setting when κ is treated as an $O(1)$-constant. Zhang et al. (2020) proposed a stabilized smoothed GDA algorithm that achieves a better complexity for the nonconvex-concave problem. Fiez & Ratliff (2021); Jin et al. (2020) provided local and global asymptotic results showing that GDA converges to a local minimax point of nonconvex-nonconcave minimax problem almost surely. We note that all of this previous work has not addressed the non-asymptotic convergence rates of finding local minimax points. It was not until very recently that Luo et al. (2022); Chen et al. (2021b) proposed (inexact) cubic-regularized Newton methods for solving this problem; these are second-order algorithms that provably converge to a local minimax point. These algorithms are limited, however, to minimax optimization and cannot be used to solve the more general bilevel optimization problems.

Organization. The rest of this work is organized as follows. Section 2 delineates the assumptions and specific algorithmic subroutines. Section 3 formally presents the RAHGD algorithm along with a complexity bound for finding approximation first-order stationary points. Section 4 proposes the PRAHGD, the perturbed version of RAHGD, along with its complexity bound for

Algorithm 1 AGD$(h, z_0, T, \alpha, \beta)$

Input: objective $h(\cdot)$; initialization z_0; iteration number $T \geq 1$; step-size $\alpha > 0$; momentum param. $\beta \in (0, 1)$
$\tilde{z}_0 \leftarrow z_0$
for $t = 0, \ldots, T-1$ **do**
  $z_{t+1} \leftarrow \tilde{z}_t - \alpha \nabla h(\tilde{z}_t)$
  $\tilde{z}_{t+1} \leftarrow z_{t+1} + \beta(z_{t+1} - z_t)$
end for
Output: z_T

finding approximate second-order stationary points. Section 5 presents PRAHGD applied to minimax optimization. Section 6 concludes the paper and discusses future directions. Presentations of technical analysis and empirical studies are deferred to the supplementary materials.

Notation. We let $\|\cdot\|_2$ be the spectral norm of matrices and the Euclidean norm of vectors. Given a real symmetric matrix A, we let $\lambda_{\max}(A)$ ($\lambda_{\min}(A)$) denote its largest (smallest) eigenvalue, and also $\kappa(A) = \lambda_{\max}(A)/\lambda_{\min}(A)$ denote the condition number. We use the notation $\mathbb{B}(r)$ to present the closed Euclidean ball with radius r centered at the origin. We denote $Gc(f, \epsilon)$, $JV(f, \epsilon)$ and $HV(f, \epsilon)$ as the oracle complexities of gradients, Jacobian-vector products and Hessian-vector products, respectively. Finally, for two positive sequences $\{a_n\}$ and $\{b_n\}$ we denote $a_n = \Omega(b_n)$ (resp. $a_n = \mathcal{O}(b_n)$) if $a_n \geq Cb_n$ (resp. $a_n \leq Cb_n$) for all n, and also $a_n = \Theta(b_n)$ if both $a_n = \Omega(b_n)$ and $a_n = \mathcal{O}(b_n)$ hold for some absolute constant $C > 0$, and $\widetilde{\mathcal{O}}(\cdot)$ or $\widetilde{\Omega}(\cdot)$ is adopted in turn when C incorporates a polylogarithmic factor in problem parameters.

2 Preliminaries

In this section, we first proceed to establish convergence of the algorithmic subroutines related to our algorithm—*accelerated gradient descent* and the *conjugate gradient method*. Then, we present the notation and assumptions necessary for our problem setting. We proceed to establish convergence of these two algorithmic subroutines in the following paragraphs.

Subroutine 1: Accelerated Gradient Descent. Our first component is *Nesterov's accelerated gradient descent* (AGD), which is an acceleration of the first-order method in smooth convex optimization. We describe the details of AGD for minimizing a given smooth and strongly convex function in Algorithm 1, which exhibits the following *optimal* convergence rate (Nesterov, 2013):

Lemma 2.1 (Nesterov (2013))**.** *Running Algorithm 1 on an ℓ_h-smooth and μ_h-strongly convex objective function $h(\cdot)$ with $\alpha = 1/\ell_h$ and $\beta = (\sqrt{\kappa_h} - 1)/(\sqrt{\kappa_h} + 1)$ produces an output z_T satisfying*

$$\|z_T - z^*\|_2^2 \leq (1 + \kappa_h)\left(1 - \frac{1}{\sqrt{\kappa_h}}\right)^T \|z_0 - z^*\|_2^2,$$

where $z^* = \arg\min_z h(z)$ and $\kappa_h = \ell_h/\mu_h$ denotes the condition number of the objective h.

Algorithm 2 CG(A, b, T, q_0)

Input: quadratic objective (as in Eq. (5)); initialization q_0; iteration number $T \geq 1$
$r_0 \leftarrow Aq_0 - b$, $p_0 \leftarrow -r_0$
for $t = 0, \ldots, T-1$ **do**
  $\alpha_t \leftarrow \dfrac{r_t^T r_t}{p_t^T A p_t}$
  $q_{t+1} \leftarrow q_t + \alpha_t p_t$
  $r_{t+1} \leftarrow r_t + \alpha_t A p_t$
  $\beta_{t+1} \leftarrow \dfrac{r_{t+1}^T r_{t+1}}{r_t^T r_t}$
  $p_{t+1} \leftarrow -r_{t+1} + \beta_{t+1} p_t$
end for
Output: q_T

Subroutine 2: Conjugate Gradient Method. The *(linear) conjugate gradient* (CG) method was proposed by Hestenes and Stiefel in the 1950s as an iterative method for solving linear systems with positive definite coefficient matrices. It serves as an alternative to Gaussian elimination that is well-suited for solving large problems. CG can be formulated as the minimization of the quadratic objective function

$$\frac{1}{2} q^\top A q - q^\top b, \tag{5}$$

where $A \in \mathbb{R}^{d \times d}$ is a positive definite matrix and $b \in \mathbb{R}^d$ is a fixed vector. We summarize the setup of CG for minimizing the function (5) in Algorithm 2, and record the following convergence property (Nocedal & Wright, 2006):

Lemma 2.2 (Nocedal & Wright (2006))**.** *Running Algorithm 2 for minimizing quadratic function (5) produces q_T satisfying*

$$\|q_T - q^*\|_2 \leq 2\sqrt{\kappa_A}\left(\frac{\sqrt{\kappa_A} - 1}{\sqrt{\kappa_A} + 1}\right)^T \|q_0 - q^*\|_2,$$

where $q^* = A^{-1}b$ denotes the unique minimizer of Eq. (5), and $\kappa_A = \lambda_{\max}(A)/\lambda_{\min}(A)$ denotes the condition number of (positive definite) matrix A.[3]

[3]When minimizing the quadratic objective equation (5), CG and AGD enjoy comparable convergence speeds. In fact in squared Euclidean metric, Lemma 2.2 implies a conver-

Table 1: Comparison of complexities for nonconvex bilevel optimization algorithms of finding approximate FOSPs.

Algorithm	$Gc(f,\epsilon)$	$Gc(g,\epsilon)$	$JV(g,\epsilon)$	$HV(g,\epsilon)$
BA (Ghadimi & Wang, 2018)	$\mathcal{O}(\kappa^4\epsilon^{-2})$	$\mathcal{O}(\kappa^5\epsilon^{-2.5})$	$\mathcal{O}(\kappa^4\epsilon^{-2})$	$\tilde{\mathcal{O}}(\kappa^{4.5}\epsilon^{-2})$
AID-BiO (Ji et al., 2021)	$\mathcal{O}(\kappa^3\epsilon^{-2})$	$\mathcal{O}(\kappa^4\epsilon^{-2})$	$\mathcal{O}(\kappa^3\epsilon^{-2})$	$\mathcal{O}(\kappa^{3.5}\epsilon^{-2})$
ITD-BiO (Ji et al., 2021)	$\mathcal{O}(\kappa^3\epsilon^{-2})$	$\tilde{\mathcal{O}}(\kappa^4\epsilon^{-2})$	$\tilde{\mathcal{O}}(\kappa^4\epsilon^{-2})$	$\tilde{\mathcal{O}}(\kappa^4\epsilon^{-2})$
`RAHGD` (this work)	$\tilde{\mathcal{O}}(\kappa^{2.75}\epsilon^{-1.75})$	$\tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$	$\tilde{\mathcal{O}}(\kappa^{2.75}\epsilon^{-1.75})$	$\tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$

Table 2: Comparison of complexities for nonconvex bilevel optimization algorithms of finding approximate SOSPs.

Algorithm	$Gc(f,\epsilon)$	$Gc(g,\epsilon)$	$JV(g,\epsilon)$	$HV(g,\epsilon)$
Perturbed AID (Huang et al., 2022)	$\tilde{\mathcal{O}}(\kappa^3\epsilon^{-2})$	$\tilde{\mathcal{O}}(\kappa^4\epsilon^{-2})$	$\tilde{\mathcal{O}}(\kappa^3\epsilon^{-2})$	$\tilde{\mathcal{O}}(\kappa^{3.5}\epsilon^{-2})$
`PRAHGD` (this work)	$\tilde{\mathcal{O}}(\kappa^{2.75}\epsilon^{-1.75})$	$\tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$	$\tilde{\mathcal{O}}(\kappa^{2.75}\epsilon^{-1.75})$	$\tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$

— Notation $\tilde{\mathcal{O}}$ omits a polylogarithmic factor in relevant parameters. κ: condition number of the lower-level objective.
— $Gc(f,\epsilon)$ and $Gc(g,\epsilon)$: number of gradient evaluations w.r.t. f and g.
— $JV(g,\epsilon)$: number of Jacobian-vector products $\nabla^2_{xy}g(x,y)v$.
— $HV(g,\epsilon)$: number of Hessian-vector products $\nabla^2_{yy}g(x,y)v$.

In the rest of this section we impose the following assumptions on the upper-level function f and the lower-level function g. We then turn to the details of our theoretical analysis:

Assumption 2.3. The upper-level function $f(x,y)$ and lower-level function $g(x,y)$ satisfy the following conditions:

(i) Function $g(x,y)$ is three times differentiable and μ-strongly convex with respect to y for any fixed x;

(ii) Function $f(x,y)$ is twice differentiable and M-Lipschitz continuous with respect to y;

(iii) Gradient $\nabla f(x,y)$ and $\nabla g(x,y)$ are ℓ-Lipschitz continuous with respect to x and y;

(iv) The Jacobians $\nabla^2_{xy}f(x,y)$, $\nabla^2_{xy}g(x,y)$ and Hessians $\nabla^2_{xx}f(x,y)$, $\nabla^2_{yy}f(x,y)$, $\nabla^2_{yy}g(x,y)$ are ρ-Lipschitz continuous with respect to x and y;

(v) The third-order derivatives $\nabla^3_{xyx}g(x,y), \nabla^3_{yxy}g(x,y)$ and $\nabla^3_{yyy}g(x,y)$ are ν-Lipschitz continuous with respect to x and y.

These assumptions are standard for the bilevel optimization problem we are studying. We also introduce an appropriate notion of condition number for the lower-level function $g(x,y)$.

Definition 2.4. Under Assumption 2.3, we refer to $\kappa \triangleq \ell/\mu$ the *condition number* of the lower-level objective $g(x,y)$.

Leveraging such a notion, we can show that the solution to the lower-level optimization problem $y^*(x) = \arg\min_{y\in\mathbb{R}^{d_y}} g(x,y)$ is κ-Lipschitz continuous in x under Assumption 2.3, as indicated in the following lemma:

Lemma 2.5. *Suppose Assumption 2.3 holds, then $y^*(x)$ is κ-Lipschitz continuous; that is, we have $\|y^*(x) - y^*(x')\|_2 \le \kappa \|x - x'\|_2$ for any $x, x' \in \mathbb{R}^{d_x}$.*

We also can show that $\Phi(x)$ admits Lipschitz continuous gradients and Lipschitz continuous Hessians, as shown in the following lemmas:

Lemma 2.6. *Suppose Assumption 2.3 holds, then $\Phi(x)$ is $\tilde{L}$-gradient Lipschitz continuous; that is, we have $\|\nabla\Phi(x) - \nabla\Phi(x')\| \le \tilde{L}\|x - x'\|$ for any $x, x' \in \mathbb{R}^{d_x}$, where $\tilde{L} = \mathcal{O}(\kappa^3)$.*

Lemma 2.7. *Suppose Assumption 2.3 holds, then $\Phi(x)$ is $\tilde{\rho}$-Hessian Lipschitz continuous; that is, $\|\nabla^2\Phi(x) - \nabla^2\Phi(x')\| \le \tilde{\rho}\|x - x'\|$ for any $x, x' \in \mathbb{R}^{d_x}$, where $\tilde{\rho} = \mathcal{O}(\kappa^5)$.*

The detailed form of $\tilde{L}$ and $\tilde{\rho}$ can be found in Appendix A. We give the formal definition of an ϵ-first-order stationary point as well as an (ϵ,τ)-second-order stationary point for any prescribed $\epsilon, \tau > 0$, as follows:

Definition 2.8 (Approximate first-order stationary point)**.** Under Assumption 2.3, we call x an *ϵ-first-order stationary point* of $\Phi(x)$ if $\|\nabla\Phi(x)\|_2 \le \epsilon$.

Definition 2.9 (Approximate second-order stationary point)**.** Under Assumption 2.3, we call x an *(ϵ,τ)-second-order stationary point* of $\Phi(x)$ if $\|\nabla\Phi(x)\|_2 \le \epsilon$ and $\lambda_{\min}(\nabla^2\Phi(x)) \ge -\tau$.

gence rate of $\|q_T - q^*\|_2^2 \le 4\kappa_A \exp\left(-\frac{4}{\sqrt{\kappa_A}+1}\cdot T\right)\|q_0 - q^*\|_2^2$ and hence running CG instead of AGD for equation (5) improves the coefficient in the exponent by an asymptotic factor of four while maintaining the $\mathcal{O}(\kappa_A)$-prefactor up to a numerical constant. Our two algorithmic subroutines AGD and CG are logically connected, and our adoption of CG whenever possible is partly due to its additional advantage of requiring fewer input parameters (corresponding to α, β in Algorithm 1).

Algorithm 3 (Perturbed) Restarted Accelerated HyperGradient Descent, (P)RAHGD

Input: initial vector $x_{0,0}$; step-size $\eta > 0$; momentum parameter $\theta \in (0,1)$; parameters $\alpha > 0, \beta \in (0,1)$; parameter $\{T_{t,k}\}$ of AGD; parameter $\{T'_{t,k}\}$ of CG; iteration threshold $K \geq 1$; parameter B for triggering restarting; perturbation radius $r > 0$; option Perturbation $\in \{0,1\}$

$k \leftarrow 0,\ t \leftarrow 0,\ x_{0,-1} \leftarrow x_{0,0}$

$y_{0,-1} \leftarrow \mathrm{AGD}\left(g(x_{0,-1}, \cdot), 0, T_{0,-1}, \alpha, \beta\right)$

$v_{0,-1} \leftarrow y_{0,-1}$

while $k < K$

  $w_{t,k} \leftarrow x_{t,k} + (1-\theta)(x_{t,k} - x_{t,k-1})$

  $y_{t,k} \leftarrow \mathrm{AGD}(g(w_{t,k}, \cdot), y_{t,k-1}, T_{t,k}, \alpha, \beta)$

  $v_{t,k} \leftarrow \mathrm{CG}(\nabla^2_{yy} g(w_{t,k}, y_{t,k}), \nabla_y f(w_{t,k}, y_{t,k}), T'_{t,k}, v_{t,k-1})$

  $u_{t,k} \leftarrow \nabla_x f(w_{t,k}, y_{t,k}) - \nabla^2_{xy} g(w_{t,k}, y_{t,k}) v_{t,k}$

  $x_{t,k+1} \leftarrow w_{t,k} - \eta u_{t,k}$

  $k \leftarrow k+1$

  if $k \sum_{i=0}^{k-1} \|x_{t,i+1} - x_{t,i}\|^2 > B^2$

    $v_{t+1,-1} \leftarrow v_{t,k}$

    if Perturbation $= 0$

      $x_{t+1,0} \leftarrow x_{t,k}$

    else

      $x_{t+1,0} \leftarrow x_{t,k} + \xi_{t,k}$ with $\xi_{t,k} \sim \mathrm{Unif}(\mathbb{B}(r))$

    end if

    $x_{t+1,-1} \leftarrow x_{t+1,0}$

    $k \leftarrow 0,\ t \leftarrow t+1$

    $y_{t,-1} \leftarrow \mathrm{AGD}(g(x_{t,-1}, \cdot), 0, T_{t,-1}, \alpha, \beta)$

  end if

end while

$K_0 \leftarrow \arg\min_{\lfloor \frac{K}{2} \rfloor \leq k \leq K-1} \|x_{t,k+1} - x_{t,k}\|_2$

Output: $\hat{w} \leftarrow \frac{1}{K_0+1} \sum_{k=0}^{K_0} w_{t,k}$

We remark that these concepts are commonly used in the nonconvex optimization literature (Nesterov & Polyak, 2006). The approximate second-order stationary point is sometimes referred to as an "approximate local minimizer." With these preliminaries in hand, we are ready to proceed with a description of the (perturbed) restarted accelerated hypergradient descent method.

3 Restarted Accelerated HyperGradient Descent Algorithm

In this section, we present our *restarted accelerated hypergradient descent* (RAHGD) algorithm and provide corresponding upper bounds for query complexity. We present the details of RAHGD in Algorithm 3, which has a nested loop structure. The outer loop, indexed by k, uses the accelerated gradient descent method to find the solver of (1a). The AGD step in Line 7 is used to find the inexact solver of (1b). The CG step is added to compute the Hessian-vector product, as shown in (2). We note that the iteration numbers of the AGD and CG steps play an important role in the convergence analysis of Algorithm 3; moreover, at the end of this section we will show that the total iteration number of AGD and CG can be bounded sharply. Finally, note that there is a restarting step in Line 17.

We let subscript t index the times of restarting. We note that the subscript t of epoch number is added in Algorithm 3 purely for the sake of an easier convergence analysis. The incurred storage of iterations across all epochs can be avoided when implementing Algorithm 3 in practice.

In accelerated nonconvex optimization, a straightforward application of AGD cannot ensure consistent decrements of the objective function. Inspired by the work of Li & Lin (2022), we add a restarting step in Line 17—we define $\mathcal{K}$ to be the iteration number when the "if condition" triggers, and hence the iterates from $k = 0$ to $k = \mathcal{K}$ constructs one single epoch, where $\mathcal{K} = \min_k \left\{k \geq 1 : k \sum_{t=0}^{k-1} \|x_{t+1} - x_t\|_2^2 > B^2\right\}$. Then we can have the objective function consistently decrease with respect to each epoch when we run Algorithm 3. We provide the convergence results for RAHGD in the rest of this section.

Denote $v_k^* = \left(\nabla^2_{yy} g(w_k, y_k)\right)^{-1} \nabla_y f(w_k, y_k)$. Due to the bilevel optimization problem we are considering we impose the following conditions on the inexact gradient. Recall that the overall objective function $\Phi(x)$ is $\tilde{L}$-gradient Lipschitz continuous, and both the upper-level function $f(x,y)$ and the lower-level function $g(x,y)$ are ℓ-gradient Lipschitz continuous:

Condition 3.1. *Let $w_{-1} = x_{-1}$. Then for some $\sigma > 0$, we assume that the estimators $y_k \in \mathbb{R}^{d_y}$ and $v_k \in \mathbb{R}^{d_y}$ satisfy the conditions*

$$\|y_k - y^*(w_k)\|_2 \leq \frac{\sigma}{2\tilde{L}}, \quad \text{for each } k = -1, 0, 1, 2, \ldots \tag{6}$$

and

$$\|v_k - v_k^*\| \leq \frac{\sigma}{2\ell}, \quad \text{for each } k = 0, 1, 2, \ldots \tag{7}$$

Remark 3.2. We will show at the end of this section that Condition 3.1 is guaranteed to hold after running AGD and CG for a sufficient number of iterates.

Under Condition 3.1, the bias of $\hat{\nabla}\Phi(x_k)$ defined in equation (4) can be bounded as shown in the following lemma:

Lemma 3.3 (Inexact gradients)**.** *Suppose Assumption 2.3 and Condition 3.1 hold, then we have $\|\nabla\Phi(w_k) - \hat{\nabla}\Phi(w_k)\|_2 \leq \sigma$.*

In the following theorem we show that the iteration complexity in the outer loop is bounded.

Theorem 3.4 (RAHGD finding ϵ-FOSP)**.** *Suppose that Assumptions 2.3 and Condition 3.1 hold. Let*

$$\eta = \frac{1}{4\tilde{L}}, \quad B = \sqrt{\frac{\epsilon}{\tilde{\rho}}}, \quad \theta = 4(\tilde{\rho}\epsilon\eta^2)^{1/4}, \quad K = \frac{1}{\theta},$$
$$\alpha = \frac{1}{\ell}, \quad \beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}, \quad \sigma = \epsilon^2,$$

and assume that $\epsilon \leq \frac{\tilde{L}^2}{\tilde{\rho}}$. *Denote* $\Delta = \Phi(x_{\text{int}}) - \min_x \Phi(x)$. *Then* RAHGD *in Algorithm 3 terminates within* $\mathcal{O}(\Delta\tilde{L}^{0.5}\tilde{\rho}^{0.25}\epsilon^{-1.75})$ *iterates, outputting* $\hat{w}$ *satisfying* $\|\nabla\Phi(\hat{w})\|_2 \leq 83\epsilon$.

Theorem 3.4 says that Algorithm 3 can find an ϵ-first-order stationary point with $\mathcal{O}(\kappa^{2.75}\epsilon^{-1.75})$ iterations in the outer loop. The following result indicates that Condition 3.1 holds if we run AGD and CG for a sufficient number of iterations. In addition, the total number of iterations in one epoch is at most $\mathcal{O}(\kappa^{0.5}\mathcal{K}\log(1/\epsilon))$:

Proposition 3.5. *Suppose Assumption 2.3 holds. In the t-th epoch, we set the inner loop iteration number* $T_{t,k}$ *and the CG iteration number* $T'_{t,k}$. *We run Algorithm 3 with the parameter chosen in Theorem 3.4. Then all* $y_{t,k}$ *and* $v_{t,k}$ *satisfy Condition 3.1. For each t, we also have the following control for the inner loops:* $\sum_{k=-1}^{\mathcal{K}-1} T_{t,k} \leq \mathcal{O}(\kappa^{0.5}\mathcal{K}\log(1/\epsilon))$ *and* $\sum_{k=0}^{\mathcal{K}-1} T'_{t,k} \leq \mathcal{O}(\kappa^{0.5}\mathcal{K}\log(1/\epsilon))$.

The detailed forms of $T_{t,k}$ and $T'_{t,k}$ can be found in Appendix B. Combined with Theorem 3.4, we finally obtain the total number of oracle calls as follows:

Corollary 3.6 (Oracle complexity of RAHGD finding ϵ-FOSP)**.** *Under Assumption 2.3, we run* RAHGD *in Algorithm 3 with the parameters set as in Theorem 3.4 and Proposition 3.5. The output* $\hat{w}$ *is then an* ϵ*-first-order stationary point of* $\Phi(x)$. *Additionally, the oracle complexities satisfy* $Gc(f,\epsilon) = \tilde{\mathcal{O}}(\kappa^{2.75}\epsilon^{-1.75})$, $Gc(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$, $JV(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{2.75}\epsilon^{-1.75})$ *and* $HV(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$.

The algorithm can be adapted to solving the single-level nonconvex minimization problem where κ reduces to 1, and the given complexity matches the state-of-the-art (Carmon et al., 2018; Agarwal et al., 2017; Carmon et al., 2017; Jin et al., 2018; Li & Lin, 2022). The best known lower bound in this setting is $\Omega(\epsilon^{-1.714})$ (Carmon et al., 2021). Closing this $O(\epsilon^{-0.036})$-gap remains open even in nonconvex minimization settings.

4 Perturbed Restarted Accelerated HyperGradient Descent Algorithm

In this section, we introduce perturbation to our RAHGD algorithm. In many nonconvex problems encountered in practice in machine learning, most first-order stationary points presented are saddle points (Dauphin et al., 2014; Lee et al., 2019; Jin et al., 2017). Recall that the notion of second-order stationary points consists of not only zero gradient value, but positive semidefinite Hessian matrix as well. Earlier work of Jin et al. (2018); Li & Lin (2022) shows that one can obtain an approximate second-order stationary point by intermittently *perturbing* the algorithm using random noise. We present the details of our *perturbed restarted accelerated hypergradient descent* (PRAHGD) in Algorithm 3. Compared with RAHGD, a noise-perturbation step is added in Algorithm 3 [Line 17, option `Perturbation` = 1].

We proceed with the complexity analysis for PRAHGD, where we show that PRAHGD in Algorithm 3 outputs an $(\epsilon, \sqrt{\tilde{\rho}\epsilon}\,)$-second-order stationary point within $\tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$ oracle queries:

Theorem 4.1 (PRAHGD finding $(\epsilon, O(\sqrt{\epsilon}))$-SOSP)**.** *Suppose that Assumption 2.3 and Condition 3.1 hold. Let*

$$\chi = \mathcal{O}\left(\log\frac{d_x}{\zeta\epsilon}\right), \ \eta = \frac{1}{4\tilde{L}}, \ K = \frac{2\chi}{\theta}, \ B = \frac{1}{288\chi^2}\sqrt{\frac{\epsilon}{\tilde{\rho}}},$$
$$\theta = \frac{1}{2}(\tilde{\rho}\epsilon\eta^2)^{1/4}, \ \sigma = \min\left\{\frac{\tilde{\rho}B\zeta r\theta}{2\sqrt{d_x}}, \epsilon^2\right\}, \ \alpha = \frac{1}{\ell},$$
$$\beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}, \ r = \min\left\{\frac{\tilde{L}B^2}{4C}, \frac{B+B^2}{\sqrt{2}}, \frac{\theta B}{20K}, \sqrt{\frac{\theta B^2}{2K}}\right\},$$

for some positive constant C, where we assume that $\epsilon \leq \frac{\tilde{L}^2}{\tilde{\rho}}$. *Denote* $\Delta = \Phi(x_{\text{int}}) - \min_{x\in\mathbb{R}^{d_x}} \Phi(x)$. *Then* PRAHGD *in Algorithm 3 terminates in at most* $\mathcal{O}\big(\Delta\tilde{L}^{0.5}\tilde{\rho}^{0.25}\chi^6\cdot\epsilon^{-1.75}\big)$ *iterations and the output satisfies* $\|\nabla\Phi(\hat{w})\|_2 \leq \epsilon$ *and* $\lambda_{\min}(\nabla^2\Phi(\hat{w})) \geq -1.011\sqrt{\tilde{\rho}\epsilon}$ *with probability at least* $1-\zeta$.

Theorem 4.1 says that PRAHGD in Algorithm 3 can find an $(\epsilon, \sqrt{\tilde{\rho}\epsilon}\,)$-second-order stationary point within $\tilde{\mathcal{O}}(\kappa^{2.75}\epsilon^{-1.75})$ iterations in the outer loop. The following proposition shows that Condition 3.1 holds in this setting. In addition, the total number of iterations in one epoch is at most $\mathcal{O}(\kappa^{0.5}\,\mathcal{K}\log(1/\epsilon))$ (we remind the reader that $\mathcal{K}$ denotes the iteration number of one single epoch, as introduced in Section 3):

Proposition 4.2. *Suppose Assumption 2.3 holds. In the t-th epoch, we set the inner loop iteration number* $T_{t,k}$ *and the CG iteration number* $T'_{t,k}$. *We run Algorithm 3 with the parameters chosen in Theorem 4.1. Then all* $y_{t,k}$ *and* $v_{t,k}$ *satisfy the Condition 3.1. For each t, we also have the following control for the inner loops:* $\sum_{k=-1}^{\mathcal{K}-1} T_{t,k} \leq \mathcal{O}\left(\kappa^{0.5}\mathcal{K}\log(1/\epsilon)\right)$ *and* $\sum_{k=0}^{\mathcal{K}-1} T'_{t,k} \leq \mathcal{O}\left(\kappa^{0.5}\mathcal{K}\log(1/\epsilon)\right)$.

The detailed form of $T_{t,k}$ and $T'_{t,k}$ can be found in Appendix C. Combining this result with Theorem 4.1, we finally obtain the total number of gradient oracle calls as follows:

Corollary 4.3 (Oracle complexity of PRAHGD finding $(\epsilon, O(\sqrt{\epsilon}))$-SOSP)**.** *Under Assumption 2.3, we run* PRAHGD *in Algorithm 3 with all parameters set as in Theorem 4.1. The output $\hat{w}$ is then an $\big(\epsilon, \sqrt{\rho\epsilon}\big)$-second-order stationary point of $\Phi(x)$. Additionally, the oracle complexities satisfy that $Gc(f,\epsilon) = \tilde{\mathcal{O}}(\kappa^{2.75}\epsilon^{-1.75})$, $Gc(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$, $JV(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{2.75}\epsilon^{-1.75})$ and $HV(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$.*

We remark that the listed oracle-call query complexities are identical to the corresponding ones in Corollary 3.6 of Section 3, up to a polylogarithmic factor, indicating that the perturbed version imposes essentially no extra cost while allowing the avoidance of saddle points.

5 Improved Convergence for Accelerating Minimax Optimization

This section applies the ideas of PRAHGD to find approximate second-order stationary points in minimax optimization problem of the form

$$\min_{x\in\mathbb{R}^{d_x}} \left\{ \bar{\Phi}(x) \triangleq \max_{y\in\mathbb{R}^{d_y}} \bar{f}(x,y) \right\}, \tag{8}$$

where $\bar{f}(x,y)$ is strongly concave in y but possibly nonconvex in x. Problems of form (8) can be regarded as a special case of a bilevel optimization problem by taking $f(x,y) = \bar{f}(x,y)$ and $g(x,y) = -\bar{f}(x,y)$. Danskin's theorem yields $\nabla\bar{\Phi}(x) = \nabla_x \bar{f}(x, y^*(x))$ in this case, which is consistent with a hypergradient of form (2) with the optimality condition for the lower-level problem invoked; that is, $\nabla_y f(x, y^*(x)) = 0$. This implies that when applying PRAHGD to the minimax optimization problem (8), *no* CG subroutine is called and *no* Jacobian-vector or Hessian-vector product operation is invoked.

We first show in Lemma 5.1 that the minimax problem enjoys tighter Lipschitz continuity parameters than the general bilevel problem:

Lemma 5.1. *Suppose that $\bar{f}(x,y)$ is ℓ-smooth, ρ-Hessian Lipschitz continuous with respect to x and y and μ-strongly concave in y but possibly nonconvex in x. Then the objective $\bar{\Phi}(x)$ is $(\kappa+1)\ell$-smooth and admits $(4\sqrt{2}\kappa^3\rho)$-Lipschitz continuous Hessians.*

We formally introduce the *perturbed restarted accelerated gradient descent ascent* (PRAGDA) as in Algorithm 4 (see Appendix D). Utilizing the PRAHGD complexity result as in Theorems 4.1 and 4.2 together with Lemma 5.1, we can take $\tilde{L} = (\kappa+1)\ell$ and $\tilde{\rho} = 4\sqrt{2}\kappa^3\rho$ to conclude an improved oracle complexity upper bounds for finding second-order stationary points for this particular problem, indicated by the following result:

Theorem 5.2 (Oracle complexity of PRAGDA finding $(\epsilon, O(\sqrt{\epsilon}))$-SOSP)**.** *Under the settings of Lemma 5.1, Algorithm 4 outputs an $\big(\epsilon, \mathcal{O}(\kappa^{1.5}\sqrt{\epsilon})\big)$-second-order stationary point of $\bar{\Phi}(x)$ in equation (8) within $\tilde{\mathcal{O}}(\kappa^{1.75}\epsilon^{-1.75})$ gradient oracle calls.*

Prior to this work, the state-of-the-art algorithm was attained by the *inexact minimax cubic Newton* (iMCN) method (Luo et al., 2022), which under comparable settings outputs an $\big(\epsilon, \mathcal{O}(\kappa^{1.5}\sqrt{\epsilon})\big)$-approximate SOSP within oracle queries of $\tilde{\mathcal{O}}(\kappa^2\epsilon^{-1.5})$ gradients, $\tilde{\mathcal{O}}(\kappa^{1.5}\epsilon^{-2})$ Hessian-vector products and $\tilde{\mathcal{O}}(\kappa\epsilon^{-2})$ Jacobian-vector products. We compare the query complexity upper bound of PRAGDA with iMCN in detail. As can be observed, the total oracle complexity of PRAGDA is no worse than that of iMCN since $\tilde{\mathcal{O}}(\kappa^{1.75}\epsilon^{-1.75}) \le \tilde{\mathcal{O}}(\kappa^2\epsilon^{-1.5} + \kappa^{1.5}\epsilon^{-2})$, a simple application of AM-GM inequality. Moreover, PRAGDA only requires gradient oracle calls while iMCN additionally requires Hessian-vector and Jacobian-vector oracle calls. To summarize, PRAGDA enjoys an oracle complexity that is not inferior to that of iMCN, whereas in both of the regimes $\kappa \gg \epsilon^{-1}$ and $\kappa \ll \epsilon^{-1}$ PRAGDA's complexity is strictly superior.

6 Conclusion

We have presented the *Restarted Accelerated HyperGradient Descent* (RAHGD) method for solving nonconvex-strongly-convex bilevel optimization problems. Our accelerated method is able to find an ϵ-first-order stationary point of the objective within $\tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$ oracle complexity, where κ is the condition number of the lower-level objective and ϵ is the desired accuracy. Furthermore, we have proposed a perturbed variant of RAHGD for finding an $\big(\epsilon, \mathcal{O}(\kappa^{2.5}\sqrt{\epsilon})\big)$-second-order stationary point within the same order of oracle complexity up to a polylogarithmic factor. As a byproduct, our algorithm variant PRAGDA improves upon the existing upper complexity bound for finding second-order stationary points in nonconvex-strongly-concave minimax optimization problems. Important directions for future research include extending our results to the nonconvex-convex setting and stochastic setting in bilevel optimization and also minimax optimization as its special case.

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Accelerating Inexact HyperGradient Descent for Bilevel Optimization Supplementary Materials

A Basic Lemmas

In this section, we provide some basic lemmas.

Lemma A.1. *Suppose Assumption 2.3 holds, then $y^*(x)$ is κ-Lipschitz continuous, that is,*

$$\|y^*(x) - y^*(x')\|_2 \leq \kappa \|x - x'\|_2$$

for any $x, x' \in \mathbb{R}^{d_x}$.

Proof. Recall that

$$y^*(x) = \arg\min_{y \in \mathbb{R}^{d_y}} g(x, y).$$

The optimality condition leads to $\nabla_y g(x, y^*(x)) = 0$ for each $x \in \mathbb{R}^{d_x}$. By taking a further derivative with respect to x on both sides and applying the chain rule (Rudin, 1976), we obtain

$$\nabla^2_{yx} g(x, y^*(x)) + \nabla^2_{yy} g(x, y^*(x)) \frac{\partial y^*(x)}{\partial x} = 0.$$

The smoothness and strong convexity of g in y immediately indicate

$$\frac{\partial y^*(x)}{\partial x} = -(\nabla^2_{yy} g(x, y^*(x)))^{-1} \nabla^2_{yx} g(x, y^*(x)) \ .$$

Thus we have

$$\left\| \frac{\partial y^*(x)}{\partial x} \right\|_2 = \left\| (\nabla^2_{yy} g(x, y^*(x)))^{-1} \nabla^2_{yx} g(x, y^*(x)) \right\|_2 \leq \frac{\ell}{\mu} = \kappa \ ,$$

where the inequality is based on the fact that $g(x, y)$ is ℓ-smooth with respect to x and y and μ-strongly convex with respect to y for any x.

Therefore, we proved that $y^*(x)$ is κ-Lipschitz continuous. □

We also can show that $\Phi(x)$ admits Lipschitz continuous gradients and Lipschitz continuous Hessians, as shown in the following lemmas:

Lemma A.2. *Suppose Assumption 2.3 holds, then $\Phi(x)$ is $\tilde{L}$-gradient Lipschitz continuous, that is,*

$$\|\nabla \Phi(x) - \nabla \Phi(x')\| \leq \tilde{L} \|x - x'\|$$

for any $x, x' \in \mathbb{R}^{d_x}$, where

$$\tilde{L} = \ell + \frac{2\ell^2 + \rho M}{\mu} + \frac{\ell^3 + 2\rho\ell M}{\mu^2} + \frac{\rho \ell^2 M}{\mu^3} \ .$$

Proof. Recall that

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

We denote $\mathcal{H}_1(x) = \nabla_x f(x, y^*(x))$, $\mathcal{H}_2(x) = \nabla^2_{xy} g(x, y^*(x))$, $\mathcal{H}_3(x) = \big(\nabla^2_{yy} g(x, y^*(x))\big)^{-1}$ and $\mathcal{H}_4(x) = \nabla_y f(x, y^*(x))$, then

$$\nabla\Phi(x) = \mathcal{H}_1(x) - \mathcal{H}_2(x)\mathcal{H}_3(x)\mathcal{H}_4(x) \ .$$

We first consider $\mathcal{H}_1(x),\ \mathcal{H}_2(x)$ and $\mathcal{H}_4(x)$. For any $x,\ x' \in \mathbb{R}^{d_x}$, we have

$$\begin{aligned} \|\mathcal{H}_1(x) - \mathcal{H}_1(x')\| &\le \ell(\|x - x'\| + \|y^*(x) - y^*(x')\|) \\ &\le \ell(1+\kappa)\|x - x'\| \ , \end{aligned}$$

where we use triangle inequality in the first inequality and Lemma A.2 in the second one.

We also have

$$\begin{aligned} \|\mathcal{H}_2(x) - \mathcal{H}_2(x')\| &\le \rho(\|x - x'\| + \|y^*(x) - y^*(x')\|) \\ &\le \rho(1+\kappa)\|x - x'\| \end{aligned}$$

and

$$\begin{aligned} \|\mathcal{H}_4(x) - \mathcal{H}_4(x')\| &\le \ell(\|x - x'\| + \|y^*(x) - y^*(x')\|) \\ &\le \ell(1+\kappa)\|x - x'\|. \end{aligned}$$

We next consider $\mathcal{H}_3(x)$. For any $x,\ x' \in \mathbb{R}^{d_x}$, we have

$$\begin{aligned} &\|\mathcal{H}_3(x) - \mathcal{H}_3(x')\| \\ &\quad= \left\| \big(\nabla^2_{yy} g(x, y^*(x))\big)^{-1} - \big(\nabla^2_{yy} g(x', y^*(x'))\big)^{-1} \right\| \\ &\quad\le \left\| \big(\nabla^2_{yy} g(x, y^*(x))\big)^{-1} \right\| \left\| \nabla^2_{yy} g(x', y^*(x')) - \nabla^2_{yy} g(x, y^*(x)) \right\| \left\| \big(\nabla^2_{yy} g(x', y^*(x'))\big)^{-1} \right\| \\ &\quad\le \frac{1}{\mu^2} \rho(\|x - x'\| + \|y^*(x) - y^*(x')\|) \\ &\quad\le \frac{\rho(1+\kappa)}{\mu^2} \|x - x'\| \ . \end{aligned}$$

We also have

$$\|\mathcal{H}_2(x)\| \le \ell, \quad \|\mathcal{H}_3(x)\| \le \frac{1}{\mu} \quad \text{and} \quad \|\mathcal{H}_4(x)\| \le M.$$

for any $x \in \mathbb{R}^{d_x}$. Then for any $x,\ x' \in \mathbb{R}^{d_x}$ we have

$$\begin{aligned} &\|\nabla\Phi(x) - \nabla\Phi(x')\| \\ &\quad\le \|\mathcal{H}_1(x) - \mathcal{H}_1(x')\| + \|\mathcal{H}_2(x)\mathcal{H}_3(x)\mathcal{H}_4(x) - \mathcal{H}_2(x')\mathcal{H}_3(x')\mathcal{H}_4(x')\| \\ &\quad\le \ell(1+\kappa)\|x - x'\| + \|\mathcal{H}_2(x)\mathcal{H}_3(x)\mathcal{H}_4(x) - \mathcal{H}_2(x)\mathcal{H}_3(x)\mathcal{H}_4(x')\| \\ &\qquad + \|\mathcal{H}_2(x)\mathcal{H}_3(x)\mathcal{H}_4(x') - \mathcal{H}_2(x)\mathcal{H}_3(x')\mathcal{H}_4(x')\| \\ &\qquad + \|\mathcal{H}_2(x)\mathcal{H}_3(x')\mathcal{H}_4(x') - \mathcal{H}_2(x')\mathcal{H}_3(x')\mathcal{H}_4(x')\| \\ &\quad\le \ell(1+\kappa)\|x - x'\| + \|\mathcal{H}_2(x)\|\|\mathcal{H}_3(x)\|\|\mathcal{H}_4(x) - \mathcal{H}_4(x')\| \\ &\qquad + \|\mathcal{H}_2(x)\|\|\mathcal{H}_4(x')\|\|\mathcal{H}_3(x) - \mathcal{H}_3(x')\| \\ &\qquad + \|\mathcal{H}_3(x')\|\|\mathcal{H}_4(x')\|\|\mathcal{H}_2(x) - \mathcal{H}_2(x')\| \\ &\quad\le \ell(1+\kappa)\|x - x'\| + \frac{\ell^2}{\mu}(1+\kappa)\|x - x'\| + \frac{\ell\rho M}{\mu^2}(1+\kappa)\|x - x'\| + \frac{M\rho}{\mu}(1+\kappa)\|x - x'\| \\ &\quad= \left(\ell + \frac{2\ell^2 + \rho M}{\mu} + \frac{\ell^3 + 2\rho\ell M}{\mu^2} + \frac{\rho\ell^2 M}{\mu^3}\right) \|x - x'\| \ . \end{aligned}$$

□

Lemma A.3. *(Huang et al., 2022, Lemma 3.4). Suppose Assumption 2.3 holds, then $\Phi(x)$ is $\tilde{\rho}$-Hessian Lipschitz continuous, that is, $\|\nabla^2\Phi(x) - \nabla^2\Phi(x')\| \le \tilde{\rho}\|x - x'\|$ for any $x, x' \in \mathbb{R}^{d_x}$, where*

$$\tilde{\rho} = \left[\left(\rho + \frac{2\ell\rho + M\nu}{\mu} + \frac{2M\ell\nu + \rho\ell^2}{\mu^2} + \frac{M\ell^2\nu}{\mu^3}\right)\left(1 + \frac{\ell}{\mu}\right) + \left(\frac{2\ell\rho}{\mu} + \frac{4M\rho^2 + 2\ell^2\rho}{\mu^2} + \frac{2M\ell\rho^2}{\mu^3}\right)\left(1 + \frac{\ell}{\mu}\right)^2 + \left(\frac{M\rho^2}{\mu^2} + \frac{\rho\ell}{\mu}\right)\left(1 + \frac{\ell}{\mu}\right)^3\right] .$$

Lemma A.4 (Inexact gradients)**.** *Suppose Assumption 2.3 and Condition 3.1 hold, then we have*

$$\|\nabla\Phi(w_k) - \hat{\nabla}\Phi(w_k)\|_2 \le \sigma .$$

Proof. Recall that

$$\nabla\Phi(x) = \nabla_x f(x, y^*(x)) - \nabla^2_{xy} g(x, y^*(x))\big(\nabla^2_{yy} g(x, y^*(x))\big)^{-1}\nabla_y f(x, y^*(x))$$

and

$$\hat{\nabla}\Phi(x_k) = \nabla_x f(x_k, y_k) - \nabla^2_{xy} g(x_k, y_k) v_k .$$

We define

$$\bar{\nabla}\Phi(x_k) = \nabla_x f(x_k, y_k) - \nabla^2_{xy} g(x_k, y_k)\big(\nabla^2_{yy} g(x_k, y_k)\big)^{-1}\nabla_y f(x_k, y_k) ,$$

then we have

$$\begin{aligned}
||\nabla\Phi(w_k) - \hat{\nabla}\Phi(w_k)||_2 &= ||\nabla\Phi(w_k) - \bar{\nabla}\Phi(w_k) + \bar{\nabla}\Phi(w_k) - \hat{\nabla}\Phi(w_k)||_2 \\
&\le ||\nabla\Phi(w_k) - \bar{\nabla}\Phi(w_k)||_2 + ||\bar{\nabla}\Phi(w_k) - \hat{\nabla}\Phi(w_k)||_2 \\
&\le \tilde{L}||y_k - y^*(w_k)||_2 + \ell\left|\left|v_k - \big(\nabla^2_{yy} g(w_k, y_k)\big)^{-1}\nabla_y f(w_k, y_k)\right|\right|_2 \\
&\le \sigma ,
\end{aligned}$$

where we use the triangle inequality in the first inequality, Lemma 2.6 and Assumption 2.3(c) in the second inequality and Condition 3.1 in the last one. □

Lemma A.5. *(Luo et al., 2022, Lemmas 1 and 3) Assume that $\bar{f}(x, y)$ is ℓ-smooth, ρ-Hessian Lipschitz continuous with respect to x and y and μ-strongly concave in y but possibly nonconvex in x, then the objective $\bar{\Phi}(x)$ is $(\kappa + 1)\ell$-smooth and $(4\sqrt{2}\kappa^3\rho)$-Hessian Lipschitz continuous.*

B Proofs in Section 3

In this section, we provide the proofs for the theorems in Section 3. We separate our proof into three parts. We first prove that $\Phi(x)$ decreases by at least $\Omega(\epsilon^{3/2})$ in one epoch and thus the total number of epochs is bounded. Then we show that our `RAHGD` in Algorithm 3 can output an ϵ-FOSP. Finally, we provide the oracle calls complexity analysis.

B.1 Proof of Theorem 3.4

To prove Theorem 3.4 we primarily consider the algorithmic behavior in a single epoch; the desired result then follows by a simple recursive argument. We omit the subscript t for notational simplicity. For each epoch except the final one, we have $1 \le \mathcal{K} \le K$,

$$\mathcal{K}\sum_{i=0}^{\mathcal{K}-1} \|x_{i-1} - x_i\|_2^2 > B^2, \tag{9}$$

$$\|x_k - x_0\|_2^2 \le k\sum_{i=0}^{k-1} \|x_{i+1} - x_i\|_2^2 \le B^2, \qquad \forall k < \mathcal{K}, \tag{10}$$

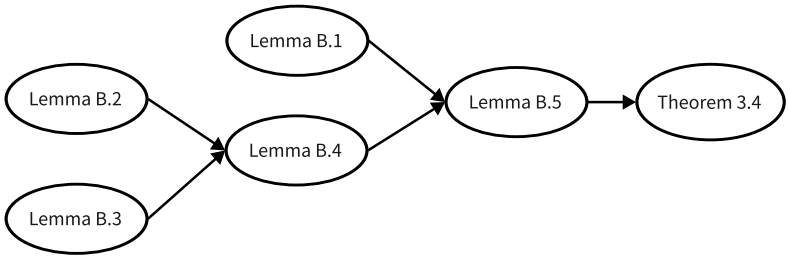


Figure 1: Proof process for Theorem 3.4

$$\|w_k - x_0\|_2 \le \|x_k - x_0\|_2 + \|x_k - x_{k-1}\|_2 \le 2B, \qquad \forall k < \mathcal{K}, \tag{11}$$
$$\|w_k - w_{k-1}\|_2 \le 2B, \qquad \forall k < \mathcal{K}, \tag{12}$$

where equation (12) can be proved by induction as follows. For $k = 0$, we have

$$\|w_0 - w_{-1}\|_2 = 0 \le 2B.$$

For $k = 1$, we have

$$\|w_1 - w_0\|_2 = \|(x_1 - x_0) + (1-\theta)(x_1 - x_0)\|_2 \le 2B.$$

For $k \ge 2$, we have

$$\begin{aligned}\|w_k - w_{k-1}\|_2 &\le (2-\theta)\|x_k - x_{k-1}\|_2 + (1-\theta)\|x_{k-1} - x_{k-2}\|_2 \\ &\le 2\sqrt{2\|x_k - x_{k-1}\|_2^2 + 2\|x_{k-1} - x_{k-2}\|_2^2} \le 2B.\end{aligned}$$

In the last epoch, the "if condition" does not trigger and the while loop breaks until $k = K$. Hence, we have

$$\|x_k - x_0\|_2^2 \le k\sum_{i=0}^{k-1}\|x_{i+1} - x_i\|_2^2 \le B^2, \qquad \forall k \le K, \tag{13}$$
$$\|w_k - x_0\|_2 \le 2B, \qquad \forall k \le K. \tag{14}$$

In the sequel, we first present five introductory lemmas, namely Lemmas B.1— B.5, and then prove our main Theorem 3.4. Lemma B.1 captures how $\Phi(x)$ decreases within an epoch in the case of large gradients. When the gradient is small, we utilize quadratic functions to approximate $\Phi(x)$ as shown in Lemma B.2 and Lemma B.3 and then further we introduce Lemma B.4 which illustrates how $\Phi(x)$ decreases in the small gradient case. Combining Lemma B.1 and Lemma B.4 we can introduce Lemma B.5 which shows that the total number of epochs is bounded since $\Phi(x)$ is bounded below. Finally we are ready to prove Theorem 3.4. Figure 1 provides a pictorial description of our proof strategy.

We first consider the case when $\|\nabla\Phi(w_{\mathcal{K}-1})\|_2$ is large in the following lemma.

Lemma B.1. *Suppose that Assumption 2.3 and Condition 3.1 hold. Let $\eta \le \frac{1}{4\tilde{L}}$ and $0 \le \theta \le 1$. When the "if condition" triggers and $\|\nabla\Phi(w_{\mathcal{K}-1})\|_2 > \frac{B}{\eta}$, we have*

$$\Phi(x_{\mathcal{K}}) - \Phi(x_0) \le -\frac{B^2}{4\eta} + \sigma B + \frac{5\eta\sigma^2\mathcal{K}}{8}\ .$$

Proof. Since $\Phi(x)$ has $\tilde{L}$-Lipschitz continuous gradient, we have

$$\begin{aligned}\Phi(x_{k+1}) &\le \Phi(w_k) + \langle\nabla\Phi(w_k), x_{k+1} - w_k\rangle + \frac{\tilde{L}}{2}\|x_{k+1} - w_k\|_2^2 \\ &\le \Phi(w_k) - \eta\langle\nabla\Phi(w_k), \hat{\nabla}\Phi(w_k)\rangle + \frac{\eta}{8}\|\hat{\nabla}\Phi(w_k)\|_2^2\ ,\end{aligned}$$

where we use $\eta \leq \frac{1}{4\tilde{L}}$. We also have

$$\Phi(x_k) \geq \Phi(w_k) + \langle \nabla\Phi(w_k), x_k - w_k\rangle - \frac{\tilde{L}}{2}\|x_k - w_k\|_2^2 \ .$$

Combining the above inequalities leads to

$$\begin{aligned}
&\Phi(x_{k+1}) - \Phi(x_k) \\
&\leq -\langle \nabla\Phi(w_k), x_k - w_k\rangle + \frac{\tilde{L}}{2}\|x_k - w_k\|_2^2 - \eta\langle \nabla\Phi(w_k), \hat{\nabla}\Phi(w_k)\rangle + \frac{\eta}{8}\|\hat{\nabla}\Phi(w_k)\|_2^2 \\
&= \frac{1}{\eta}\langle x_{k+1} - w_k, x_k - w_k\rangle + \langle \hat{\nabla}\Phi(w_k) - \nabla\Phi(w_k), x_k - w_k\rangle + \frac{\tilde{L}}{2}\|x_k - w_k\|_2^2 \\
&\qquad - \eta\langle \nabla\Phi(w_k), \hat{\nabla}\Phi(w_k)\rangle + \frac{\eta}{8}\|\hat{\nabla}\Phi(w_k)\|_2^2 \\
&= \frac{1}{2\eta}\left(\|x_{k+1} - w_k\|_2^2 + \|x_k - w_k\|_2^2 - \|x_{k+1} - x_k\|_2^2\right) + \langle \hat{\nabla}\Phi(w_k) - \nabla\Phi(w_k), x_k - w_k\rangle \\
&\qquad + \frac{\tilde{L}}{2}\|x_k - w_k\|_2^2 - \eta\langle \nabla\Phi(w_k), \hat{\nabla}\Phi(w_k)\rangle + \frac{\eta}{8}\|\hat{\nabla}\Phi(w_k)\|_2^2 \\
&\overset{(a)}{\leq} \frac{5}{8\eta}\|x_k - w_k\|_2^2 - \frac{1}{2\eta}\|x_{k+1} - x_k\|_2^2 + \langle \hat{\nabla}\Phi(w_k) - \nabla\Phi(w_k), x_k - w_k\rangle + \frac{5\eta}{8}\|\hat{\nabla}\Phi(w_k)\|_2^2 \\
&\qquad - \eta\langle \nabla\Phi(w_k), \hat{\nabla}\Phi(w_k)\rangle \\
&\overset{(b)}{\leq} \frac{5}{8\eta}\|x_k - x_{k-1}\|_2^2 - \frac{1}{2\eta}\|x_{k+1} - x_k\|_2^2 + \|\hat{\nabla}\Phi(w_k) - \nabla\Phi(w_k)\|_2 \cdot \|x_k - x_{k-1}\|_2 \\
&\qquad + \frac{5\eta}{8}\|\hat{\nabla}\Phi(w_k)\|_2^2 - \eta\langle \nabla\Phi(w_k), \hat{\nabla}\Phi(w_k)\rangle \\
&= \frac{5}{8\eta}\|x_k - x_{k-1}\|_2^2 - \frac{1}{2\eta}\|x_{k+1} - x_k\|_2^2 + \|\hat{\nabla}\Phi(w_k) - \nabla\Phi(w_k)\|_2 \cdot \|x_k - x_{k-1}\|_2 \\
&\qquad + \frac{5\eta}{8}\|\hat{\nabla}\Phi(w_k)\|_2^2 - \frac{\eta}{2}\left(\|\nabla\Phi(w_k)\|_2^2 + \left\|\hat{\nabla}\Phi(w_k)\right\|_2^2 - \left\|\nabla\Phi(w_k) - \hat{\nabla}\Phi(w_k)\right\|_2^2\right) \\
&\overset{(c)}{\leq} \frac{5}{8\eta}\|x_k - x_{k-1}\|_2^2 - \frac{1}{2\eta}\|x_{k+1} - x_k\|_2^2 + \|\hat{\nabla}\Phi(w_k) - \nabla\Phi(w_k)\|_2 \cdot \|x_k - x_{k-1}\|_2 \\
&\qquad - \frac{3\eta}{8}\left\|\nabla\Phi(w_k)\right\|_2^2 + \frac{5\eta}{8}\left\|\nabla\Phi(w_k) - \hat{\nabla}\Phi(w_k)\right\|_2^2 \\
&\overset{(d)}{\leq} \frac{5}{8\eta}\|x_k - x_{k-1}\|_2^2 - \frac{1}{2\eta}\|x_{k+1} - x_k\|_2^2 - \frac{3\eta}{8}\left\|\nabla\Phi(w_k)\right\|_2^2 + \sigma\|x_k - x_{k-1}\|_2 + \frac{5\eta}{8}\sigma^2 \ ,
\end{aligned}$$

where we use $\tilde{L} \leq \frac{1}{4\eta}$ in $\overset{(a)}{\leq}$, $\|x_k - w_k\|_2 = (1-\theta)\|x_k - x_{k-1}\|_2 \leq \|x_k - x_{k-1}\|_2$ in $\overset{(b)}{\leq}$, the triangle inequality in $\overset{(c)}{\leq}$ and Lemma 3.3 in $\overset{(d)}{\leq}$.

Summing over the above inequality with $k = 0, 1, \cdots, \mathcal{K}-1$ and using $x_0 = x_{-1}$, we have

$$\begin{aligned}
&\Phi(x_{\mathcal{K}}) - \Phi(x_0) && (15)\\
&\leq \frac{1}{8\eta}\sum_{k=0}^{\mathcal{K}-2}\|x_{k+1} - x_k\|_2^2 - \frac{3\eta}{8}\sum_{k=0}^{\mathcal{K}-1}\|\nabla\Phi(w_k)\|_2^2 + \sigma\sum_{k=0}^{\mathcal{K}-1}\|x_k - x_{k-1}\|_2 + \frac{5\eta\sigma^2\mathcal{K}}{8} && (16)\\
&\overset{(e)}{\leq} \frac{1}{8\eta}\sum_{k=0}^{\mathcal{K}-2}\|x_{k+1} - x_k\|_2^2 - \frac{3\eta}{8}\sum_{k=0}^{\mathcal{K}-1}\|\nabla\Phi(w_k)\|_2^2 + \sigma\sqrt{\mathcal{K}-1}\sqrt{\sum_{k=0}^{\mathcal{K}-2}\|x_{k+1} - x_k\|_2^2} + \frac{5\eta\sigma^2\mathcal{K}}{8} && (17)\\
&\overset{(f)}{\leq} \frac{B^2}{8\eta} - \frac{3\eta}{8}\left\|\nabla\Phi(w_{\mathcal{K}-1})\right\|_2^2 + \sigma B + \frac{5\eta\sigma^2\mathcal{K}}{8} && (18)\\
&\overset{(g)}{\leq} -\frac{B^2}{4\eta} + \sigma B + \frac{5\eta\sigma^2\mathcal{K}}{8} \ , && (19)
\end{aligned}$$

where we use the Cauchy-Schwarz inequality in $\overset{(e)}{\leq}$, the "if condition" in $\overset{(f)}{\leq}$ and $\|\nabla\Phi(w_{\mathcal{K}-1})\|_2 > \frac{B}{\eta}$ in $\overset{(g)}{\leq}$. □

Now we consider the case when $\|\nabla\Phi(w_{\mathcal{K}-1})\|_2$ is small.

If $\|\nabla\Phi(w_{\mathcal{K}-1})\|_2 \leq \frac{B}{\eta}$, then equation (11) and Lemma 3.3 lead to

$$\begin{aligned}\|x_{\mathcal{K}} - x_0\|_2 &\leq \|w_{\mathcal{K}-1} - x_0\|_2 + \eta\|\nabla\Phi(w_{\mathcal{K}-1})\|_2 + \eta\left\|\hat{\nabla}\Phi(w_{\mathcal{K}-1}) - \nabla\Phi(w_{\mathcal{K}-1})\right\|_2 \\ &\leq 3B + \eta\sigma.\end{aligned}$$

For the epoch initialized at x_0, we denote $\mathbf{H} = \nabla^2\Phi(x_0)$, and eigen-decompose this matrix as $\mathbf{H} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$ with $\mathbf{\Lambda} \in \mathbb{R}^{d_x \times d_x}$ being orthogonal and $\mathbf{U} \in \mathbb{R}^{d_x \times d_x}$ being diagonal. Let λ_j be the j-th eigenvalue of $\mathbf{H}$. We denote $\tilde{x} = \mathbf{U}^T x, \tilde{w} = \mathbf{U}^T w$ and $\tilde{\nabla}\Phi(w) = \mathbf{U}^T\nabla\Phi(w)$. Let $\tilde{x}^j$ and $\tilde{\nabla}^j\Phi(w)$ be the j-th coordinate of $\tilde{x}$ and $\tilde{\nabla}\Phi(w)$, respectively. Since Φ admits $\tilde{\rho}$-Lipschitz continuous Hessian, we have

$$\begin{aligned}\Phi(x_{\mathcal{K}}) - \Phi(x_0) &\leq \langle\nabla\Phi(x_0), x_{\mathcal{K}} - x_0\rangle + \frac{1}{2}(x_{\mathcal{K}} - x_0)^\top\mathbf{H}(x_{\mathcal{K}} - x_0) + \frac{\tilde{\rho}}{6}\|x_{\mathcal{K}} - x_0\|_2^3 \\ &= \langle\tilde{\nabla}\Phi(x_0), \tilde{x}_{\mathcal{K}} - \tilde{x}_0\rangle + \frac{1}{2}(\tilde{x}_{\mathcal{K}} - \tilde{x}_0)^\top\mathbf{\Lambda}(\tilde{x}_{\mathcal{K}} - \tilde{x}_0) + \frac{\tilde{\rho}}{6}\|x_{\mathcal{K}} - x_0\|_2^3 \\ &\leq \phi(\tilde{x}_{\mathcal{K}}) - \phi(\tilde{x}_0) + \frac{\tilde{\rho}}{6}(3B + \eta\sigma)^3,\end{aligned} \tag{20}$$

where we denote

$$\phi(x) = \langle\tilde{\nabla}\Phi(x_0), x - \tilde{x}_0\rangle + \frac{1}{2}(x - \tilde{x}_0)^\top\mathbf{\Lambda}(x - \tilde{x}_0),$$

and

$$\phi_j(x) = \langle\tilde{\nabla}^j\Phi(x_0), x - \tilde{x}_0^j\rangle + \frac{1}{2}\lambda_j(x - \tilde{x}_0^j)^2.$$

Let

$$\tilde{\delta}_k^j = (\mathbf{U}^\top\hat{\nabla}\Phi(w_k))^j - \nabla\phi_j(\tilde{w}_k^j) \quad \text{and} \quad \tilde{\delta}_k = \mathbf{U}^\top\hat{\nabla}\Phi(w_k) - \nabla\phi(\tilde{w}_k)\ ,$$

then the iteration of the algorithm means

$$\tilde{w}_k^j = \tilde{x}_k^j + (1-\theta)(\tilde{x}_k^j - \tilde{x}_{k-1}^j), \tag{21}$$

and

$$\tilde{x}_{k+1}^j = \tilde{w}_k^j - \eta(\mathbf{U}^\top\hat{\nabla}\Phi(w_k))^j = \tilde{w}_k^j - \eta\nabla\phi_j(\tilde{w}_k^j) - \eta\tilde{\delta}_k^j. \tag{22}$$

For any $k < \mathcal{K}$, we can bound $\|\tilde{\delta}_k\|_2$ as follows

$$\begin{aligned}\|\tilde{\delta}_k\| &= \left\|\mathbf{U}^\top\hat{\nabla}\Phi(w_k) - \tilde{\nabla}\Phi(w_k) + \tilde{\nabla}\Phi(w_k) - \nabla\phi(\tilde{w}_k)\right\|_2 \\ &\leq \left\|\tilde{\nabla}\Phi(w_k) - \tilde{\nabla}\Phi(x_0) - \mathbf{\Lambda}(\tilde{w}_k - \tilde{x}_0)\right\|_2 + \left\|\mathbf{U}^\top\hat{\nabla}\Phi(w_k) - \tilde{\nabla}\Phi(w_k)\right\|_2 \\ &= \|\nabla\Phi(w_k) - \nabla\Phi(x_0) - \mathbf{H}(w_k - x_0)\|_2 + \left\|\hat{\nabla}\Phi(w_k) - \nabla\Phi(w_k)\right\|_2 \\ &\leq \left\|\int_0^1\langle\nabla^2\Phi(x_0 + t(w_k - x_0)) - \mathbf{H}, w_k - x_0\rangle\,\mathrm{d}t\right\|_2 + \sigma \\ &\leq \frac{\tilde{\rho}}{2}\|w_k - x_0\|_2^2 + \sigma \\ &\leq 2\tilde{\rho}B^2 + \sigma,\end{aligned}$$

where the first inequality uses the triangle inequality, the second one is based on Lemma 3.3, the third one is based on the Lipschitz continuity of Hessian, and the last one uses equation (11).

Notice that quadratic function $\phi(x)$ equals to the sum of d_x scalar functions $\phi_j(x^j)$. Then we decompose $\phi(x)$ into $\sum_{j\in S_1}\phi_j(x^j)$ and $\sum_{j\in S_2}\phi_j(x^j)$, where

$$S_1 = \left\{ j : \lambda_j \geq -\frac{\theta}{\eta} \right\} \qquad \text{and} \qquad S_2 = \left\{ j : \lambda_j < -\frac{\theta}{\eta} \right\} .$$

We first consider the term $\sum_{j\in S_1}\phi_j(x^j)$ in the following lemma.

Lemma B.2. *Suppose that Assumption 2.3 and Condition 3.1 hold. Let $\eta \leq \frac{1}{4\tilde{L}}$ and $0 \leq \theta \leq 1$. When the "if condition" triggers and $\|\nabla\Phi(w_{\mathcal{K}-1})\|_2 \leq \frac{B}{\eta}$, then we have*

$$\sum_{j\in S_1}\phi_j(\tilde{x}^j_{\mathcal{K}}) - \sum_{j\in S_1}\phi_j(\tilde{x}^j_0) \leq -\sum_{j\in S_1}\frac{3\theta}{8\eta}\sum_{k=0}^{\mathcal{K}-1}|\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2 + \frac{2\eta\mathcal{K}}{\theta}(2\tilde{\rho}B^2+\sigma)^2 \ . \tag{23}$$

Proof. Since $\phi_j(x)$ is quadratic, we have

$$\begin{aligned}
&\phi_j(\tilde{x}^j_{k+1}) \\
&= \phi_j(\tilde{x}^j_k) + \langle \nabla\phi_j(\tilde{x}^j_k), \tilde{x}^j_{k+1}-\tilde{x}^j_k\rangle + \frac{\lambda_j}{2}|\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2 \\
&\overset{(a)}{=} \phi_j(\tilde{x}^j_k) - \frac{1}{\eta}\langle \tilde{x}^j_{k+1}-\tilde{w}^j_k+\eta\tilde{\delta}^j_k, \tilde{x}^j_{k+1}-\tilde{x}^j_k\rangle + \langle \nabla\phi_j(\tilde{x}^j_k)-\nabla\phi_j(\tilde{w}^j_k), \tilde{x}^j_{k+1}-\tilde{x}^j_k\rangle \\
&\qquad + \frac{\lambda_j}{2}|\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2 \\
&= \phi_j(\tilde{x}^j_k) - \frac{1}{\eta}\langle \tilde{x}^j_{k+1}-\tilde{w}^j_k, \tilde{x}^j_{k+1}-\tilde{x}^j_k\rangle - \langle \tilde{\delta}^j_k, \tilde{x}^j_{k+1}-\tilde{x}^j_k\rangle + \lambda_j\langle \tilde{x}^j_k-\tilde{w}^j_k, \tilde{x}^j_{k+1}-\tilde{x}^j_k\rangle \\
&\qquad + \frac{\lambda_j}{2}|\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2 \\
&= \phi_j(\tilde{x}^j_k) + \frac{1}{2\eta}\left(|\tilde{x}^j_k-\tilde{w}^j_k|^2 - |\tilde{x}^j_{k+1}-\tilde{w}^j_k|^2 - |\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2\right) - \langle \tilde{\delta}^j_k, \tilde{x}^j_{k+1}-\tilde{x}^j_k\rangle \\
&\qquad + \frac{\lambda_j}{2}\left(|\tilde{x}^j_{k+1}-\tilde{w}^j_k|^2 - |\tilde{x}^j_k-\tilde{w}^j_k|^2\right) \\
&\leq \phi_j(\tilde{x}^j_k) + \frac{1}{2\eta}\left(|\tilde{x}^j_k-\tilde{w}^j_k|^2 - |\tilde{x}^j_{k+1}-\tilde{w}^j_k|^2 - |\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2\right) + \frac{1}{2\alpha}|\tilde{\delta}^j_k|^2 + \frac{\alpha}{2}|\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2 \\
&\qquad + \frac{\lambda_j}{2}\left(|\tilde{x}^j_{k+1}-\tilde{w}^j_k|^2 - |\tilde{x}^j_k-\tilde{w}^j_k|^2\right),
\end{aligned}$$

where we use equation (21) in $\overset{(a)}{=}$.

Using the fact $\tilde{L} \geq \lambda_j \geq -\frac{\theta}{\eta}$ for $j \in S_1$ and

$$\left(-\frac{1}{2\eta}+\frac{\lambda_j}{2}\right)|\tilde{x}^j_{k+1}-\tilde{w}^j_k|^2 \leq \left(-2\tilde{L}+\frac{\tilde{L}}{2}\right)|\tilde{x}^j_{k+1}-\tilde{w}^j_k|^2 \leq 0,$$

we have

$$\begin{aligned}
&\phi_j(\tilde{x}^j_{k+1}) \\
&\leq \phi_j(\tilde{x}^j_k) + \frac{1}{2\eta}\left(|\tilde{x}^j_k-\tilde{w}^j_k|^2 - |\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2\right) + \frac{1}{2\alpha}|\tilde{\delta}^j_k|^2 + \frac{\alpha}{2}|\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2 + \frac{\theta}{2\eta}|\tilde{x}^j_k-\tilde{w}^j_k|^2 \\
&\overset{(b)}{=} \phi_j(\tilde{x}^j_k) + \frac{(1-\theta)^2(1+\theta)}{2\eta}|\tilde{x}^j_k-\tilde{x}^j_{k-1}|^2 - \left(\frac{1}{2\eta}-\frac{\alpha}{2}\right)|\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2 + \frac{1}{2\alpha}|\tilde{\delta}^j_k|^2 \\
&= \phi_j(\tilde{x}^j_k) + \frac{(1-\theta)^2(1+\theta)}{2\eta}\left(|\tilde{x}^j_k-\tilde{x}^j_{k-1}|^2 - |\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2\right) \\
&\qquad - \left(\frac{1}{2\eta}-\frac{\alpha}{2}-\frac{(1-\theta)^2(1+\theta)}{2\eta}\right)|\tilde{x}^j_{k+1}-\tilde{x}^j_k|^2 + \frac{1}{2\alpha}|\tilde{\delta}^j_k|^2
\end{aligned}$$

$$\overset{(c)}{\leq} \phi_j(\tilde{x}_k^j) + \frac{(1-\theta)^2(1+\theta)}{2\eta}\left(|\tilde{x}_k^j - \tilde{x}_{k-1}^j|^2 - |\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2\right) - \frac{3\theta}{8\eta}|\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2 + \frac{2\eta}{\theta}|\tilde{\delta}_k^j|^2$$

for each $j \in S_1$, where we use equation (22) in $\overset{(b)}{=}$ and let $\alpha = \frac{\theta}{4\eta}$ in $\overset{(c)}{\leq}$ which leads to

$$\frac{1}{2\eta} - \frac{\alpha}{2} - \frac{(1-\theta)^2(1+\theta)}{2\eta} = \frac{1}{2\eta} - \frac{\theta}{8\eta} - \frac{(1-\theta)^2(1+\theta)}{2\eta} = \frac{3\theta}{8\eta} + \frac{\theta^2-\theta^3}{2\eta} \geq \frac{3\theta}{8\eta}.$$

Summing this result over $k = 0, 1, \cdots, \mathcal{K}-1$ for $j \in S_1$ and using $x_0 = x_{-1}$, we have

$$\begin{aligned}
&\sum_{j\in S_1} \phi_j(\tilde{x}_{\mathcal{K}}^j) \\
&\leq \sum_{j\in S_1} \phi_j(\tilde{x}_0^j) - \sum_{j\in S_1} \frac{3\theta}{8\eta} \sum_{k=0}^{\mathcal{K}-1} |\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2 + \frac{2\eta}{\theta} \sum_{k=0}^{\mathcal{K}-1} \left\|\tilde{\delta}_k\right\|_2^2 - \frac{(1-\theta)^2(1+\theta)}{2\eta}|\tilde{x}_{\mathcal{K}}^j - \tilde{x}_{\mathcal{K}-1}^j|^2 \\
&\leq \sum_{j\in S_1} \phi_j(\tilde{x}_0^j) - \sum_{j\in S_1} \frac{3\theta}{8\eta} \sum_{k=0}^{\mathcal{K}-1} |\tilde{x}_{k+1}^j - \tilde{x}_k^j| + \frac{2\eta\mathcal{K}}{\theta}(2\tilde{\rho}B^2 + \sigma)^2.
\end{aligned}$$

This completes the proof. □

Next, we consider the term $\sum_{j\in S_2} \phi_j(x^j)$.

Lemma B.3. *Suppose that Assumption 2.3 and Condition 3.1 hold. Let $\eta \leq \frac{1}{4\tilde{L}}$ and $0 \leq \theta \leq 1$. When the "if condition" triggers and $\|\nabla\Phi(w_{\mathcal{K}-1})\|_2 \leq \frac{B}{\eta}$, then we have*

$$\sum_{j\in S_2} \phi_j(\tilde{x}_{\mathcal{K}}^j) - \sum_{j\in S_2} \phi_j(\tilde{x}_0^j) \leq -\sum_{j\in S_2} \frac{\theta}{2\eta} \sum_{k=0}^{\mathcal{K}-1} |\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2 + \frac{\eta\mathcal{K}}{2\theta}(2\tilde{\rho}B^2 + \sigma)^2 + \frac{\eta\mathcal{K}}{2\theta}\sigma^2 \ . \tag{24}$$

Proof. We denote $\nu_j = \tilde{x}_0^j - \frac{1}{\lambda_j}\tilde{\nabla}^j\Phi(x_0)$, then $\phi_j(x)$ can be rewritten as

$$\phi_j(x) = \frac{\lambda_j}{2}\left(x - \tilde{x}_0^j + \frac{1}{\lambda_j}\tilde{\nabla}^j\Phi(x_0)\right)^2 - \frac{1}{2\lambda_j}|\tilde{\nabla}^j\Phi(x_0)|^2 = \frac{\lambda_j}{2}(x-\nu_j)^2 - \frac{1}{2\lambda_j}|\tilde{\nabla}^j\Phi(x_0)|^2 \ .$$

For each $j \in S_2 = \{j : \lambda_j < -\frac{\theta}{\eta}\}$, we have

$$\begin{aligned}
\phi_j(\tilde{x}_{k+1}^j) - \phi_j(\tilde{x}_k^j) &= \frac{\lambda_j}{2}|\tilde{x}_{k+1}^j - \nu_j|^2 - \frac{\lambda_j}{2}|\tilde{x}_k^j - \nu_j|^2 \\
&= \frac{\lambda_j}{2}|\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2 + \lambda_j\langle\tilde{x}_{k+1}^j - \tilde{x}_k^j, \tilde{x}_k^j - \nu_j\rangle \\
&\leq -\frac{\theta}{2\eta}|\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2 + \lambda_j\langle\tilde{x}_{k+1}^j - \tilde{x}_k^j, \tilde{x}_k^j - \nu_j\rangle \ .
\end{aligned} \tag{25}$$

So we only need to bound the second part. From equation (21) and equation (22), we have

$$\begin{aligned}
\tilde{x}_{k+1}^j - \tilde{x}_k^j &= \tilde{w}_k^j - \tilde{x}_k^j - \eta\nabla\phi_j(\tilde{w}_k^j) - \eta\tilde{\delta}_k^j \\
&= (1-\theta)(\tilde{x}_k^j - \tilde{x}_{k-1}^j) - \eta\lambda_j(\tilde{w}_k^j - \nu_j) - \eta\tilde{\delta}_k^j \\
&= (1-\theta)(\tilde{x}_k^j - \tilde{x}_{k-1}^j) - \eta\lambda_j(\tilde{x}_k^j - \nu_j + (1-\theta)(\tilde{x}_k^j - \tilde{x}_{k-1}^j)) - \eta\tilde{\delta}_k^j \ .
\end{aligned}$$

So for each $j \in S_2$, we have

$$
\begin{aligned}
&\langle \tilde{x}_{k+1}^j - \tilde{x}_k^j, \tilde{x}_k^j - \nu_j \rangle \\
&\quad = (1-\theta)\langle \tilde{x}_k^j - \tilde{x}_{k-1}^j, \tilde{x}_k^j - \nu_j \rangle - \eta\lambda_j |\tilde{x}_k^j - \nu_j|^2 - \eta\lambda_j(1-\theta)\langle \tilde{x}_k^j - \tilde{x}_{k-1}^j, \tilde{x}_k^j - \nu_j \rangle - \eta\langle \tilde{\delta}_k^j, \tilde{x}_k^j - \nu_j \rangle \\
&\quad \geq (1-\theta)\langle \tilde{x}_k^j - \tilde{x}_{k-1}^j, \tilde{x}_k^j - \nu_j \rangle - \eta\lambda_j |\tilde{x}_k^j - \nu_j|^2 \\
&\qquad + \frac{\eta\lambda_j(1-\theta)}{2}(|\tilde{x}_k^j - \tilde{x}_{k-1}^j|^2 + |\tilde{x}_k^j - \nu_j|^2) + \frac{\eta}{2\lambda_j(1+\theta)}|\tilde{\delta}_k^j|^2 + \frac{\eta\lambda_j(1+\theta)}{2}|\tilde{x}_k^j - \nu_j|^2 \\
&\quad = (1-\theta)\langle \tilde{x}_k^j - \tilde{x}_{k-1}^j, \tilde{x}_k^j - \nu_j \rangle + \frac{\eta\lambda_j(1-\theta)}{2}|\tilde{x}_k^j - \tilde{x}_{k-1}^j|^2 + \frac{\eta}{2\lambda_j(1+\theta)}|\tilde{\delta}_k^j|^2 \\
&\quad = (1-\theta)\langle \tilde{x}_k^j - \tilde{x}_{k-1}^j, \tilde{x}_{k-1}^j - \nu_j \rangle + (1-\theta)|\tilde{x}_k^j - \tilde{x}_{k-1}^j|^2 + \frac{\eta\lambda_j(1-\theta)}{2}|\tilde{x}_k^j - \tilde{x}_{k-1}^j|^2 + \frac{\eta}{2\lambda_j(1+\theta)}|\tilde{\delta}_k^j|^2 \\
&\quad \geq (1-\theta)\langle \tilde{x}_k^j - \tilde{x}_{k-1}^j, \tilde{x}_{k-1}^j - \nu_j \rangle + \frac{\eta}{2\lambda_j}|\tilde{\delta}_k^j|^2 \ ,
\end{aligned}
$$

where we use the fact that $\lambda_j < 0$ when $j \in S_2$ in the first inequality and the fact

$$
\left(1 + \frac{\eta\lambda_j}{2}\right)(1-\theta) \geq \left(1 - \frac{\eta\tilde{L}}{2}\right)(1-\theta) \geq 0
$$

indicates the second inequality. Then we have

$$
\begin{aligned}
&\langle \tilde{x}_{k+1}^j - \tilde{x}_k^j, \tilde{x}_k^j - \nu_j \rangle \\
&\quad \geq (1-\theta)^k \langle \tilde{x}_1^j - \tilde{x}_0^j, \tilde{x}_0^j - \nu_j \rangle + \frac{\eta}{2\lambda_j}\sum_{i=1}^{k}(1-\theta)^{k-i}|\tilde{\delta}_i^j|^2 \\
&\quad \overset{\text{(a)}}{=} -\frac{\eta}{2\lambda_j}(1-\theta)^k \langle \nabla^j\Phi(x_0), \hat{\nabla}^j\Phi(x_0) \rangle + \frac{\eta}{2\lambda_j}\sum_{i=1}^{k}(1-\theta)^{k-i}|\tilde{\delta}_i^j|^2 \\
&\quad = -\frac{\eta}{2\lambda_j}(1-\theta)^k \left(|\nabla^j\Phi(x_0)|^2 + |\hat{\nabla}^j\Phi(x_0)|^2 - |\nabla^j\Phi(x_0) - \hat{\nabla}^j\Phi(x_0)|^2\right) + \frac{\eta}{2\lambda_j}\sum_{i=1}^{k}(1-\theta)^{k-i}|\tilde{\delta}_i^j|^2 \\
&\quad \overset{\text{(b)}}{\geq} \frac{\eta}{2\lambda_j}(1-\theta)^k \left(|\nabla^j\Phi(x_0) - \hat{\nabla}^j\Phi(x_0)|^2\right) + \frac{\eta}{2\lambda_j}\sum_{i=1}^{k}(1-\theta)^{k-i}|\tilde{\delta}_i^j|^2,
\end{aligned}
$$

where we use

$$
\tilde{x}_1^j - \tilde{x}_0^j = \tilde{x}_1^j - \tilde{w}_0^j = -\eta\left(\mathbf{U}^\top\hat{\nabla}\Phi(x_0)\right)^j \quad \text{and} \quad \tilde{x}_0^j - \nu_j = -\frac{1}{\lambda_j}\tilde{\nabla}^j\Phi(x_0)
$$

in $\overset{\text{(a)}}{=}$ and $\lambda_j < 0$ in $\overset{\text{(b)}}{\geq}$. Plugging the above inequality into equation (25) and using $\lambda_j < 0$, we have

$$
\phi_j(\tilde{x}_{k+1}^j) - \phi_j(\tilde{x}_k^j) \leq -\frac{\theta}{2\eta}|\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2 + \frac{\eta}{2}(1-\theta)^k\left(|\nabla^j\Phi(x_0) - \hat{\nabla}^j\Phi(x_0)|^2\right) + \frac{\eta}{2}\sum_{i=1}^{k}(1-\theta)^{k-i}|\tilde{\delta}_i^j|^2.
$$

Summing this result over $k = 0, 1, \ldots, \mathcal{K}-1$ for $j \in S_2$, we have

$$
\begin{aligned}
&\sum_{j\in S_2}\phi_j(\tilde{x}_{\mathcal{K}}^j) - \sum_{j\in S_2}\phi_j(\tilde{x}_0^j) \\
&\quad \leq -\sum_{j\in S_2}\frac{\theta}{2\eta}\sum_{k=0}^{\mathcal{K}-1}|\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2 + \frac{\eta}{2}\left\|\nabla\Phi(x_0) - \hat{\nabla}\Phi(x_0)\right\|_2^2\sum_{k=0}^{\mathcal{K}-1}(1-\theta)^k + \frac{\eta}{2}\sum_{k=0}^{\mathcal{K}-1}\sum_{i=1}^{k}(1-\theta)^{k-i}\|\tilde{\delta}_i\|_2^2 \\
&\quad \leq -\sum_{j\in S_2}\frac{\theta}{2\eta}\sum_{k=0}^{\mathcal{K}-1}|\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2 + \frac{\eta}{2}\sigma^2\sum_{k=0}^{\mathcal{K}-1}(1-\theta)^k + \frac{\eta}{2}\sum_{k=0}^{\mathcal{K}-1}\sum_{i=1}^{k}(1-\theta)^{k-i}\|\tilde{\delta}_i\|_2^2 \\
&\quad \leq -\sum_{j\in S_2}\frac{\theta}{2\eta}\sum_{k=0}^{\mathcal{K}-1}|\tilde{x}_{k+1}^j - \tilde{x}_k^j|^2 + \frac{\eta\mathcal{K}}{2\theta}\sigma^2 + \frac{\eta\mathcal{K}}{2\theta}(2\tilde{\rho}B + \sigma)^2,
\end{aligned}
$$

which completes the proof. □

Putting Lemmas B.2 and B.3 together we can lower bound the decrement of $\Phi(x)$ in a single epoch.

Lemma B.4. *Suppose that Assumption 2.3 and Condition 3.1 hold. Let $\eta \le \frac{1}{4\tilde{L}}$ and $0 \le \theta \le 1$. When the "if condition" triggers and $\|\nabla\Phi(w_{\mathcal{K}-1})\|_2 \le \frac{B}{\eta}$, we have*

$$\Phi(x_{\mathcal{K}}) - \Phi(x_0) \le -\frac{\epsilon^{3/2}}{\sqrt{\tilde{\rho}}} \ .$$

Proof. Summing over equation (23) and equation (24), we have

$$\begin{aligned}
\phi(\tilde{x}_{\mathcal{K}}) - \phi(\tilde{x}_0) &= \sum_{j\in S_1\cup S_2} \phi_j(\tilde{x}_{\mathcal{K}}^j) - \phi_j(\tilde{x}_0^j) \\
&\le \frac{3\theta}{8\eta}\sum_{k=0}^{\mathcal{K}-1} \|\tilde{x}_{k+1} - \tilde{x}_k\|_2^2 + \frac{5\eta\mathcal{K}}{2\theta}(2\tilde{\rho}B^2+\sigma)^2 + \frac{\eta\mathcal{K}}{2\theta}\sigma^2 \qquad (26)\\
&\le -\frac{3\theta B^2}{8\eta\mathcal{K}} + \frac{5\eta\mathcal{K}}{2\theta}(2\tilde{\rho}B^2+\sigma)^2 + \frac{\eta\mathcal{K}}{2\theta}\sigma^2,
\end{aligned}$$

where we use equation (9) in the last inequality. Plugging into equation (20) and using $\mathcal{K} \le K$, we have

$$\begin{aligned}
\Phi(x_{\mathcal{K}}) - \Phi(x_0) &\le -\frac{3\theta B^2}{8\eta\mathcal{K}} + \frac{5\eta\mathcal{K}}{2\theta}(2\tilde{\rho}B^2+\sigma)^2 + \frac{\tilde{\rho}}{6}(3B+\eta\sigma)^3 + \frac{\eta\mathcal{K}}{2\theta}\sigma^2 \\
&\le -\frac{3\theta B^2}{8\eta K} + \frac{5\eta K}{2\theta}(2\tilde{\rho}B^2+\sigma)^2 + \frac{\tilde{\rho}}{6}(3B+\eta\sigma)^3 + \frac{\eta\mathcal{K}}{2\theta}\sigma^2 \qquad (27)\\
&\le -\frac{\epsilon^{3/2}}{\sqrt{\tilde{\rho}}} \ .
\end{aligned}$$

This completes the proof. □

Now we can provide an upper bound on the total number of epochs, as shown in the following lemma.

Lemma B.5. *Consider the setting of Theorem 3.4, and we run `RAHGD` in Algorithm 3. Then the algorithm terminates in at most $\Delta\sqrt{\tilde{\rho}}\epsilon^{-3/2}$ epochs.*

Proof of Lemma B.5. From Lemma B.1 and B.4, we have

$$\Phi(x_{\mathcal{K}}) - \Phi(x_0) \le -\min\left\{\frac{\epsilon^{3/2}}{\sqrt{\tilde{\rho}}}, \frac{\epsilon\tilde{L}}{\tilde{\rho}}\right\} \ . \qquad (28)$$

Notice that in Algorithm 3, we set x_0 to be the last iterate $x_{\mathcal{K}}$ in the previous epoch. Suppose the total number of epochs $N > \Delta\sqrt{\tilde{\rho}}\epsilon^{-3/2}$, then summing over all epochs we have

$$\min_{x\in\mathbb{R}^{d_x}} \Phi(x) - \Phi(x_{\text{int}}) \le -N\min\left\{\frac{\epsilon^{3/2}}{\sqrt{\tilde{\rho}}}, \frac{\epsilon\tilde{L}}{\tilde{\rho}}\right\} < -\Delta, \qquad (29)$$

leading to a contradiction. Therefore the algorithm terminates in at most $\Delta\sqrt{\tilde{\rho}}\epsilon^{-3/2}$ epochs. □

We are now prepared to finish the proof of Theorem 3.4.

Proof of Theorem 3.4. Lemma B.5 says that `RAHGD` will terminate in at most $\Delta\sqrt{\tilde{\rho}}\epsilon^{-3/2}$ epochs. Since each epoch needs at most $K = \frac{1}{2}\big(\tilde{L}^2/(\tilde{\rho}\epsilon)\big)^{1/4}$ iterations, the total number of iterations must be less than $\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\epsilon^{-7/4}$. Recall that we have $\tilde{L} = \mathcal{O}(\kappa^3)$ and $\tilde{\rho} = \mathcal{O}(\kappa^5)$, thus the total number of iterations is at most $\mathcal{O}(\kappa^{11/4}\epsilon^{-7/4})$.

Now we consider the last epoch. Denote $\tilde{w} = \mathbf{U}^\top\hat{w} = \frac{1}{K_0+1}\sum_{k=0}^{K_0}\mathbf{U}^\top w_k = \frac{1}{K_0+1}\sum_{k=0}^{K_0}\tilde{w}_k$. Since ϕ is quadratic, we have

$$\|\phi(\tilde{w})\|_2 = \left\|\frac{1}{K_0+1}\sum_{k=0}^{K_0}\nabla\phi(\tilde{w}_k)\right\|_2$$

$$
\begin{aligned}
&\overset{\text{(a)}}{=} \frac{1}{\eta(K_0+1)} \left\| \sum_{k=0}^{K_0} \left(\tilde{x}_{k+1} - \tilde{w}_k + \eta \tilde{\delta}_k \right) \right\|_2 \\
&= \frac{1}{\eta(K_0+1)} \left\| \sum_{k=0}^{K_0} \left(\tilde{x}_{k+1} - \tilde{x}_k - (1-\theta)(\tilde{x}_k - \tilde{x}_{k-1}) + \eta \tilde{\delta}_k \right) \right\|_2 \\
&\overset{\text{(b)}}{=} \frac{1}{\eta(K_0+1)} \left\| \tilde{x}_{K_0+1} - \tilde{x}_0 - (1-\theta)(\tilde{x}_{K_0} - \tilde{x}_0 + \eta \sum_{k=0}^{K_0} \tilde{\delta}_k \right\|_2 \\
&= \frac{1}{\eta(K_0+1)} \left\| \tilde{x}_{K_0+1} - \tilde{x}_{K_0} + \theta(\tilde{x}_{K_0} - \tilde{x}_0) + \eta \sum_{k=0}^{K_0} \tilde{\delta}_k \right\|_2 \\
&\leq \frac{1}{\eta(K_0+1)} \left(\|\tilde{x}_{K_0+1} - \tilde{x}_{K_0}\|_2 + \theta \|\tilde{x}_{K_0} - \tilde{x}_0\|_2 + \eta \sum_{k=0}^{K_0} \left\| \tilde{\delta}_k \right\|_2 \right) \\
&\overset{\text{(c)}}{\leq} \frac{2}{\eta K} \|\tilde{x}_{K_0+1} - \tilde{x}_{K_0}\|_2 + \frac{2\theta B}{\eta K} + 2\tilde{\rho} B^2 + \sigma,
\end{aligned}
$$

where we use equation (22) in $\overset{\text{(a)}}{=}$, $x_{-1} = x_0$ in $\overset{\text{(b)}}{=}$; $K_0 + 1 \geq \frac{K}{2}$, equation (13) and equation (14) in $\overset{\text{(c)}}{\leq}$. From $K_0 = \arg\min_{\lfloor \frac{K}{2} \rfloor \leq k \leq K-1} \|x_{k+1} - x_k\|_2$, we have

$$
\begin{aligned}
\|x_{K_0+1} - x_{K_0}\|_2^2 &\leq \frac{1}{K - \lfloor K/2 \rfloor} \sum_{k=\lfloor K/2 \rfloor}^{K-1} \|x_{k+1} - x_k\|_2^2 \leq \frac{1}{K - \lfloor K/2 \rfloor} \sum_{k=0}^{K-1} \|x_{k+1} - x_k\|_2^2 \\
&\overset{\text{(d)}}{\leq} \frac{1}{K - \lfloor K/2 \rfloor} \frac{B^2}{K} \leq \frac{2B^2}{K^2},
\end{aligned}
$$

where we use equation (13) in $\overset{\text{(d)}}{\leq}$. On the other hand, we also have

$$
\begin{aligned}
\|\nabla \Phi(\hat{w})\|_2 = \left\| \tilde{\nabla} \Phi(\hat{w}) \right\|_2 &\leq \|\nabla \phi(\tilde{w})\|_2 + \left\| \tilde{\nabla} \Phi(\hat{w}) - \nabla \phi(\tilde{w}) \right\|_2 \\
&= \|\nabla \phi(\tilde{w})\|_2 \left\| \tilde{\nabla} \Phi(\hat{w}) - \tilde{\nabla} \Phi(x_0) - \mathbf{\Lambda}(\tilde{w} - \tilde{x}_0) \right\|_2 \\
&= \|\nabla \phi(\tilde{w})\|_2 + \|\nabla \Phi(\hat{w}) - \nabla \Phi(x_0) - \mathbf{H}(\hat{w} - x_0)\|_2 \\
&\leq \|\nabla \phi(\tilde{w})\|_2 + \frac{\tilde{\rho}}{2} \|\hat{w} - x_0\|_2^2 \overset{\text{(e)}}{\leq} \|\nabla \phi(\tilde{w})\|_2 + 2\tilde{\rho} B^2 \ ,
\end{aligned}
$$

where we use $\|\hat{w} - x_0\|_2 \leq \frac{1}{K_0+1} \sum_{k=0}^{K_0} \|w_k - x_0\|_2 \leq 2B$ from equation (14) in $\overset{\text{(e)}}{\leq}$. So we have

$$
\|\nabla \Phi(\hat{w})\|_2 \leq \frac{2\sqrt{2}B}{\eta K^2} + \frac{2\theta B}{\eta K} + 4\tilde{\rho} B^2 + \sigma \leq 83\epsilon.
$$

This completes our proof of Theorem 3.4. □

B.2 Proof of Proposition 3.5

Proof. We first consider the iterations of CG in Algorithm 3 in one epoch. We set $T'_{t,k}$ as

$$
T'_{t,k} = \begin{cases} \left\lceil \frac{\sqrt{\kappa}+1}{2} \log\left(\frac{4\ell\sqrt{\kappa}}{\sigma} \left(\|v_{0,-1}\|_2 + \frac{M}{\mu} \right) \right) \right\rceil, & k = 0, \\ \left\lceil \frac{\sqrt{\kappa}+1}{2} \log\left(\frac{4\ell\sqrt{\kappa}}{\sigma} \left(\frac{\sigma}{2\ell} + \frac{2M}{\mu} \right) \right) \right\rceil, & k \geq 1. \end{cases} \tag{30}
$$

We denote

$$
v^*(x,y) = \left(\nabla_{yy}^2 g(x,y) \right)^{-1} \nabla_y f(x,y),
$$

then

$$\|v^*(x,y)\|_2 \le \frac{M}{\mu}, \quad \forall x \in \mathbb{R}^{d_x}, y \in \mathbb{R}^{d_y}.$$

We use induction to show that

$$\left\|v_{t,k} - v_{t,k}^*\right\|_2 \le \frac{\sigma}{2\ell}$$

holds for any $k \ge 0$. For $k = 0$, Lemma 2.2 straightforwardly implies that

$$\left\|v_{t,0} - v_{t,0}^*\right\|_2 \le \frac{\left\|v_{0,-1} - v_{t,0}^*\right\|_2}{\|v_{0,-1}\|_2 + M/\mu} \cdot \frac{\sigma}{2\ell} \le \frac{\sigma}{2\ell}.$$

Suppose it holds that $\left\|v_{t,k} - v_{t,k}^*\right\|_2 \le \frac{\sigma}{2\ell}$ for any $k = k' - 1$, then we have

$$\begin{aligned}
\left\|v_{t,k'} - v_{t,k'}^*\right\|_2 &\le 2\sqrt{\kappa}\left(1 - \frac{2}{1+\sqrt{\kappa}}\right)^{T'_{t,k'}} \left\|v_{t,k'-1} - v_{t,k'}^*\right\|_2 \\
&\le 2\sqrt{\kappa}\left(1 - \frac{2}{1+\sqrt{\kappa}}\right)^{T'_{t,k'}} \left(\left\|v_{t,k'-1} - v_{t,k'-1}^*\right\|_2 + \left\|v_{t,k'-1}^* - v_{t,k'}^*\right\|_2\right) \\
&\le 2\sqrt{\kappa}\left(1 - \frac{2}{1+\sqrt{\kappa}}\right)^{T'_{t,k'}} \left(\frac{\sigma}{2\ell} + \frac{2M}{\mu}\right) \le \frac{\sigma}{2\ell},
\end{aligned}$$

where the first inequality is based on Lemma 2.2, the second one uses the triangle inequality, the third one uses the definition of T'_k. Therefore, equation (7) in Condition 3.1 holds.

The total iteration count of CG in Algorithm 3 in one epoch satisfies

$$\begin{aligned}
\sum_{k=0}^{\mathcal{K}-1} T'_k &\le \mathcal{K} + \frac{\sqrt{\kappa}+1}{2}\left(\frac{2T'_0}{\sqrt{\kappa}+1} + \sum_{k=1}^{\mathcal{K}-1} \log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\frac{\sigma}{2\ell} + \frac{2M}{\mu}\right)\right)\right) \\
&= \mathcal{K} + \frac{\sqrt{\kappa}+1}{2}\left(\frac{2T'_0}{\sqrt{\kappa}+1} + (\mathcal{K}-1)\log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\frac{\sigma}{2\ell} + \frac{2M}{\mu}\right)\right)\right) \\
&= \mathcal{K} + \frac{\sqrt{\kappa}+1}{2}\mathcal{K}\left(\frac{1}{\mathcal{K}}\log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\|v_{0,-1}\|_2 + \frac{M}{\mu}\right)\right) + \left(1 - \frac{1}{\mathcal{K}}\right)\log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\frac{\sigma}{2\ell} + \frac{2M}{\mu}\right)\right)\right).
\end{aligned}$$

Now we consider the iterations of AGD in Algorithm 3.We first show the following lemma.

Lemma B.6. *Consider the setting of Theorem 3.4, and we run Algorithm 3, then we have*

$$\|y^*(w_{t,-1})\|_2 \le \hat{C}$$

for any $t > 0$, where $\hat{C} = \|y^*(x_{0,0})\|_2 + (2B + \eta\sigma + \eta C)\kappa\Delta\sqrt{\bar{\rho}}\epsilon^{-3/2}$.

Then consider the iteratons of AGD in Algorithm 3. We choose $T_{t,k}$ as

$$T_{t,k} = \begin{cases} \left\lceil 2\sqrt{\kappa}\log\left(\frac{2\tilde{L}\sqrt{\kappa}+1}{\sigma}\hat{C}\right)\right\rceil, & k = -1. \\ \left\lceil 2\sqrt{\kappa}\log\left(\frac{2\tilde{L}\sqrt{\kappa}+1}{\sigma}\left(\frac{\sigma}{2\tilde{L}} + 2\kappa B\right)\right)\right\rceil, & k \ge 0. \end{cases} \tag{31}$$

We will use induction to show that Lemma B.6 as well as equation (6) in Condition 3.1 will hold. For $t = 0$, Lemma B.6 holds trivially. Then we use induction with respect to k to prove that

$$\|y_{t,k} - y^*(w_{t,k})\|_2 \le \frac{\sigma}{2\tilde{L}}$$

holds for any $k \ge -1$. For $k = -1$, Lemma 2.1 directly implies

$$\|y_{t,-1} - y^*(w_{t,-1})\|_2 \le \frac{\left\|y^*(w_{t,-1})\right\|_2}{\hat{C}} \cdot \frac{\sigma}{2\tilde{L}} \le \frac{\sigma}{2\tilde{L}},$$

where the second inequality is based on Lemma B.6. Suppose it holds that

$$\|y_{t,k-1} - y^*(w_{t,k-1})\|_2 \leq \frac{\sigma}{2\tilde{L}}$$

for any $k \leq k' - 1$, then we have

$$\begin{aligned}
&\|y_{t,k'} - y^*(w_{t,k'})\|_2 \\
&\leq \sqrt{1+\kappa}\left(1 - \frac{1}{\sqrt{\kappa}}\right)^{T_{t,k'}/2} \|y_{t,k'-1} - y^*(w_{t,k'})\|_2 \\
&\leq \sqrt{1+\kappa}\left(1 - \frac{1}{\sqrt{\kappa}}\right)^{T_{t,k'}/2} (\|y_{t,k'-1} - y^*(w_{t,k'-1})\|_2 + \|y^*(w_{t,k'-1}) - y^*(w_{t,k'})\|_2) \\
&\leq \sqrt{1+\kappa}\left(1 - \frac{1}{\sqrt{\kappa}}\right)^{T_{t,k'}/2} \left(\frac{\sigma}{2\tilde{L}} + \kappa \|w_{t,k'-1} - w_{t,k'}\|_2\right) \\
&\leq \sqrt{1+\kappa}\left(1 - \frac{1}{\sqrt{\kappa}}\right)^{T_{t,k'}/2} \left(\frac{\sigma}{2\tilde{L}} + 2\kappa B\right) \\
&\leq \frac{\sigma}{2\tilde{L}} ,
\end{aligned}$$

where the first inequality is based on Lemma 2.1, the second one uses the triangle inequality, the third one is based on induction hypothesis and Lemma 2.5, the fourth one uses equation (12), and the last step use the definition of $T_{t,k}$. Therefore, equation (6) in Condition 3.1 holds.

Suppose Lemma B.6 and equation (6) in Condition 3.1 hold for any $t \leq t' - 1$, then we have shown that when we choose $T'_{t,k}$ as defined in equation (30), then equation (7) in Condition 3.1 can hold. Thus, from Lemma 3.3 we obtain that:

$$\|\nabla\Phi(w_{t,k}) - \hat{\nabla}\Phi(w_{t,k})\|_2 \leq \sigma . \tag{32}$$

We claim that for any t, we can find some constant C to satisfy:

$$\|\nabla\Phi(w_{t,\mathcal{K}-1})\|_2 \leq C . \tag{33}$$

Otherwise, equation (18) in Lemma B.1 shows that $\Phi(w_{t,\mathcal{K}})$ can go to $-\infty$ which contradicts the assumption $\min_{x\in\mathbf{R}^{d_x}} \Phi(x) > -\infty$.

For any epoch $t \leq t' - 1$, we have

$$\begin{aligned}
&\|x_{t,\mathcal{K}} - x_{t,0}\|_2 \\
&\quad = \|x_{t,\mathcal{K}} - x_{t,\mathcal{K}-1} + x_{t,\mathcal{K}-1} - x_{t,0}\|_2 \\
&\quad = \left\|(1-\theta)(x_{t,\mathcal{K}-1} - x_{t,\mathcal{K}-2}) - \eta\hat{\nabla}\Phi(w_{t,\mathcal{K}-1}) + x_{t,\mathcal{K}-1} - x_{t,0}\right\|_2 \\
&\quad \leq \|x_{t,\mathcal{K}-1} - x_{t,\mathcal{K}-2}\|_2 + \|x_{t,\mathcal{K}-1} - x_{t,0}\|_2 + \eta\left\|\hat{\nabla}\Phi(w_{t,\mathcal{K}-1)}\right\|_2 \\
&\quad \leq 2B + \eta\left\|\hat{\nabla}\Phi(w_{t,\mathcal{K}-1}) - \nabla\Phi(w_{t,\mathcal{K}-1}) + \nabla\Phi(w_{t,\mathcal{K}-1})\right\|_2 \\
&\quad \leq 2B + \eta\left\|\hat{\nabla}\Phi(w_{t,\mathcal{K}-1}) - \nabla\Phi(w_{t,\mathcal{K}-1})\right\|_2 + \eta\|\nabla\Phi(w_{t,\mathcal{K}-1})\|_2 \\
&\quad \leq 2B + \eta\sigma + \eta\|\nabla\Phi(w_{t,\mathcal{K}-1})\|_2 \\
&\quad \leq 2B + \eta(\sigma + C)
\end{aligned} \tag{34}$$

for some constant C. Here we use the triangle inequality in the first inequality; equation (10) in the second one; the triangle inequality again in the third one; equation (32) in the fourth one and equation (33) in the last one.

Then for t'-th epoch, we have

$$\begin{aligned}
\|y^*(w_{t',-1}) - y^*(x_{0,0})\|_2 &\leq \kappa\|w_{t',-1} - x_{0,0}\|_2 \\
&= \kappa\|x_{t',0} - x_{0,0}\|_2
\end{aligned}$$

$$
\begin{aligned}
&= \kappa \left\| x_{t'-1,\mathcal{K}} - x_{0,0} \right\|_2 \\
&\leq \kappa (\left\| x_{t'-1,0} - x_{0,0} \right\|_2 + \left\| x_{t'-1,\mathcal{K}} - x_{t'-1,0} \right\|_2) \\
&\leq \kappa (\left\| x_{t'-1,0} - x_{1,0} \right\|_2 + (2B + \eta\sigma + \eta C)) \\
&\leq (2B + \eta\sigma + \eta C)\kappa t \ ,
\end{aligned}
$$

where the first inequality is based on the Lipschitz continuous of $y^*(x)$ shown in Lemma 2.5; the second one uses the triangle inequality; the third one is based on equation (34), and the last one uses induction. Then we have

$$
\begin{aligned}
\left\| y^*(w_{t',-1}) \right\|_2 &\leq \left\| y^*(x_{0,0}) \right\|_2 + B\kappa t' \\
&\leq \left\| y^*(x_{0,0}) \right\|_2 + \frac{(2B + \eta\sigma + \eta C)\kappa\Delta\sqrt{\tilde{\rho}}}{\epsilon^{3/2}},
\end{aligned}
$$

where we use Lemma B.5 in the last inequality.

Similarly with the case $t = 0$, we use induction with respect to k again, we have that equation (6) in Condition 3.1 hold.

This also finishes the proof for Lemma B.6.

The total number of gradient calls from AGD in Algorithm 3 in one epoch satisfies

$$
\begin{aligned}
\sum_{k=-1}^{\mathcal{K}-1} T_{t,k} &\leq 2\sqrt{\kappa} \left(\frac{T_{t,-1}}{2\sqrt{\kappa}} + \sum_{k=0}^{\mathcal{K}-1} \log \left(\sqrt{\kappa+1} + \frac{4\tilde{L}\kappa\sqrt{\kappa+1}B}{\sigma} \right) \right) + \mathcal{K} + 1 \\
&= 2\sqrt{\kappa} \left(\frac{T_{t,-1}}{2\sqrt{\kappa}} + \mathcal{K} \log \left(\sqrt{\kappa+1} + \frac{4\tilde{L}\kappa\sqrt{\kappa+1}B}{\sigma} \right) \right) + \mathcal{K} + 1 \\
&= 2\sqrt{\kappa}\mathcal{K} \left(\frac{1}{\mathcal{K}} \log \left(\frac{2\tilde{L}\sqrt{\kappa+1}}{\sigma} \hat{C} \right) + \log \left(\sqrt{\kappa+1} + \frac{4\tilde{L}\kappa\sqrt{\kappa+1}B}{\sigma} \right) \right) + \mathcal{K} + 1.
\end{aligned}
$$

This completes our proof of Proposition 3.5. □

B.3 Proof of Corollary 3.6

Proof. Theorem 3.4 says that `RAHGD` can output an ϵ-FOSP within at most $\mathcal{O}\left(\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\epsilon^{-7/4}\right)$ iterations in the outer loop. Then we have

$$
Gc(f,\epsilon) = \mathcal{O}\left(\frac{\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}}{\epsilon^{7/4}}\right) \qquad \text{and} \qquad JV(g,\epsilon) = \mathcal{O}\left(\frac{\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}}{\epsilon^{7/4}}\right) .
$$

Recall that $\tilde{L} = \mathcal{O}(\kappa^3)$ and $\tilde{\rho} = \mathcal{O}(\kappa^5)$, we have

$$
Gc(f,\epsilon) = \mathcal{O}\left(\kappa^{11/4}\epsilon^{-7/4}\right) \qquad \text{and} \qquad JV(g,\epsilon) = \mathcal{O}\left(\kappa^{11/4}\epsilon^{-7/4}\right) .
$$

Gradients of $g(x,\cdot)$ and Hessian-vector products are occurred in AGD and CG respectively. Proposition 3.5 shows that we only require $\mathcal{O}\left(\sqrt{\kappa}\mathcal{K}\log(\frac{1}{\epsilon})\right)$ iterates of AGD and CG in one epoch to have Condition 3.1 hold. From Lemma B.5 we know that `RAHGD` will terminate in at most $\Delta\sqrt{\tilde{\rho}}\epsilon^{-3/2}$ epochs. Recall that $\mathcal{K} \leq K = \frac{1}{2}\big(\tilde{L}^2/(\tilde{\rho}\epsilon)\big)^{1/4}$, we have

$$
Gc(g,\epsilon) = \mathcal{O}\left(\frac{\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\kappa^{1/2}\log(1/\epsilon)}{\epsilon^{7/4}}\right) \qquad \text{and} \qquad HV(g,\epsilon) = \mathcal{O}\left(\frac{\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\kappa^{1/2}\log(1/\epsilon)}{\epsilon^{7/4}}\right) .
$$

Hiding polylogarithmic factor and plugging in $\tilde{L} = \mathcal{O}(\kappa^3)$ and $\tilde{\rho} = \mathcal{O}(\kappa^5)$, we have

$$
Gc(g,\epsilon) = \tilde{\mathcal{O}}\left(\kappa^{13/4}\epsilon^{-7/4}\right) \qquad \text{and} \qquad HV(g,\epsilon) = \tilde{\mathcal{O}}\left(\kappa^{13/4}\epsilon^{-7/4}\right) .
$$

□

C Proofs in Section 4

In this section, we provide the proofs for theorems in Section 4. We first show that the number of epochs can be bounded. Then we prove that PRAHGD can output an $(\epsilon, \sqrt{\tilde{\rho}\epsilon})$-SOSP. Finally, we provide the oracle complexity analysis.

C.1 Proof of Theorem 4.1

We will first provide two lemmas. Lemma C.1 shows that the number of epochs is bounded. Lemma C.2 is prepared to show that PRAHGD can escape saddle points with high probability. Finally we provide the proof of theorem 4.1.

Lemma C.1. *Consider the setting of Theorem 4.1, and we run Algorithm 3, then the algorithm will terminate in at most* $\mathcal{O}\left(\Delta\sqrt{\tilde{\rho}}\chi^5\epsilon^{-3/2}\right)$ *epochs.*

Proof. From the Lipschitz continuity of gradient, we have

$$\begin{aligned}\Phi(x_{t+1,0}) - \Phi(x_{t,\mathcal{K}}) &\le \langle \nabla\Phi(x_{t,\mathcal{K}}), x_{t+1,0} - x_{t,\mathcal{K}}\rangle + \frac{\tilde{L}}{2}\left\|x_{t+1,0} - x_{t,\mathcal{K}}\right\|_2^2 \\ &= \langle \nabla\Phi(x_{t,\mathcal{K}}), \xi_t\rangle + \frac{\tilde{L}}{2}\left\|\xi_t\right\|_2^2 \\ &\le \left\|\nabla\Phi(x_{t,\mathcal{K}})\right\|_2 r + \frac{\tilde{L}r^2}{2} \ .\end{aligned}$$

If $\left\|\nabla\Phi(w_{\mathcal{K}-1})\right\|_2 > \frac{B}{\eta}$, then Lemma B.1 means when the "if condition" triggers, we have

$$\Phi(x_{\mathcal{K}}) - \Phi(x_0) \le -\frac{B^2}{4\eta} + \sigma B + \frac{5\eta\sigma^2 K}{8} \ . \tag{35}$$

We say that $\left\|\nabla\Phi(x_{t,\mathcal{K}})\right\|_2$ is bounded. Otherwise, one gradient descent step $z = x_{t,\mathcal{K}} - \eta\nabla\Phi(x_{t,\mathcal{K}})$ leads to

$$\Phi(z) \le \Phi(x_{t,\mathcal{K}}) + \langle \nabla\Phi(x_{t,\mathcal{K}}), -\eta\nabla\Phi(x_{t,\mathcal{K}})\rangle + \frac{\tilde{L}\eta^2}{2}\left\|\nabla\Phi(x_{t,\mathcal{K}})\right\|_2^2 = \Phi(x_{t,\mathcal{K}}) - \frac{7\eta}{8}\left\|\nabla\Phi(x_{t,\mathcal{K}})\right\|_2^2 \ ,$$

which means $\Phi(z) \sim -\infty$ which contradicts with the assumption $\min_{x\in\mathbb{R}^{d_x}}\Phi(x) > -\infty$. Let $\left\|\nabla\Phi(x_{t,\mathcal{K}})\right\|_2 \le C$, then we have

$$\Phi(x_{t+1,0}) - \Phi(x_{t,\mathcal{K}}) \le Cr + \frac{\tilde{L}r^2}{2} \le \frac{B^2}{8\eta} \ , \tag{36}$$

where we use the definition of r in the second inequality. Summing over equation (35) and equation (36), we obtain

$$\Phi(x_{t+1,0}) - \Phi(x_{t,0}) \le -\frac{B^2}{8\eta} + \sigma B + \frac{5\eta\sigma^2 K}{8} \le -\frac{B^2}{8\eta} = -\frac{\epsilon\tilde{L}}{165888\tilde{\rho}\chi^4}$$

for all epochs. On the other hand, if $\left\|\nabla\Phi(w_{\mathcal{K}-1})\right\|_2 \le \frac{B}{\eta}$, Lemma B.4 means

$$\Phi(x_{\mathcal{K}}) - \Phi(x_0) \le -\frac{3\theta B^2}{8\eta K} + \frac{5\eta K}{2\theta}(2\tilde{\rho}B^2 + \sigma)^2 + \frac{\tilde{\rho}}{6}(3B + \eta\sigma)^3 + \frac{\eta K}{2\theta}\sigma^2.$$

We also have

$$\begin{aligned}\left\|\nabla\Phi(x_{\mathcal{K}})\right\|_2 &\le \left\|\nabla\Phi(w_{\mathcal{K}-1})\right\|_2 + \left\|\nabla\Phi(x_{\mathcal{K}}) - \nabla\Phi(w_{\mathcal{K}-1})\right\|_2 \\ &\le \left\|\nabla\Phi(w_{\mathcal{K}-1})\right\|_2 + \tilde{L}\left\|x_{\mathcal{K}} - w_{\mathcal{K}-1}\right\|_2 \\ &\le \left\|\nabla\Phi(w_{\mathcal{K}-1})\right\|_2 + \tilde{L}\eta\left(\left\|\nabla\Phi(w_{\mathcal{K}-1})\right\|_2 + \left\|\hat{\nabla}\Phi(w_{\mathcal{K}-1}) - \nabla\Phi(w_{\mathcal{K}-1})\right\|_2\right) \\ &\le \frac{B}{\eta} + \tilde{L}B + \frac{\sigma}{4} = \frac{5B}{4\eta} + \frac{\sigma}{4} \ .\end{aligned}$$

So we obtain

$$\Phi(x_{t+1,0}) - \Phi(x_{t,\mathcal{K}}) \leq \frac{5Br}{4\eta} + \frac{\sigma r}{4} + \frac{\tilde{L}r^2}{2} \leq \frac{\theta B^2}{8\eta K} + \frac{\sigma B^2}{4},$$

and

$$\begin{aligned}\Phi(x_{t+1,0}) - \Phi(x_{t,0}) &\leq -\frac{\theta B^2}{4\eta K} + \frac{5\eta K}{2\theta}(2\tilde{\rho}B^2 + \sigma)^2 + \frac{\tilde{\rho}}{6}(3B + \eta\sigma)^3 + \frac{\eta K}{2\theta}\sigma^2 + \frac{\sigma B^2}{4} \\ &\leq -\frac{\epsilon^{1.5}}{663552\sqrt{\tilde{\rho}}\chi^5}\ .\end{aligned}$$

Hence, the algorithm will terminate in at most $\mathcal{O}\left(\Delta\sqrt{\tilde{\rho}}\chi^5\epsilon^{-3/2}\right)$ epochs. □

Before proving that PRAHGD can output an $(\epsilon, \sqrt{\tilde{\rho}\epsilon}\,)$-SOSP, we first show the following lemma.

Lemma C.2. *Following the setting of Theorem 4.1, we additionally suppose that $\lambda_{\min}(\mathbf{H}) < -\sqrt{\epsilon\tilde{\rho}}$, where $\mathbf{H} = \nabla^2\Phi(x)$ for given $x \in \mathbb{R}^{d_x}$. We suppose points $x_0', x_0'' \in \mathbb{R}^{d_x}$ satisfy $\|x_0' - x\|_2 \leq r$, $\|x_0'' - x\|_2 \leq r$ and $x_0' - x_0'' = r_0 e_1$, where e_1 is the minimum eigen-direction of $\mathbf{H}$ and $r_0 = \frac{\zeta r}{\sqrt{d_x}}$. Running PRAHGD in Algorithm 3 with initialization $x_{0,0} = x_0'$ and $x_{0,0} = x_0''$, respectively, then at least one of these two initial points leads to its iterations triggering the "if condition."*

Proof. Recall that the update rule of PRAHGD can be written as:

$$x_{k+1} = (2-\theta)x_k - (1-\theta)x_{k-1} - \eta\hat{\nabla}\Phi((2-\theta)x_k - (1-\theta)x_{k-1}).$$

We denote $z_k = x_k' - x_k''$, then

$$\begin{aligned}z_{k+1} &= (2-\theta)z_k - (1-\theta)z_{k-1} - \eta(\hat{\nabla}\Phi(w_k') - \hat{\nabla}\Phi(w_k''))) \\ &= (2-\theta)(\mathbf{I} - \eta\mathbf{H} - \eta\mathbf{\Omega}_k)z_k - (1-\theta)(\mathbf{I} - \eta\mathbf{H} - \eta\mathbf{\Omega}_k)z_{k-1} - \eta(\varsigma_k - \varsigma_k'),\end{aligned}$$

where

$$\mathbf{\Omega}_k = \int_0^1 (\nabla^2\Phi(tw_k + (1-t)w_k') - K)\,\mathrm{d}t,\ \ \varsigma_k' = \nabla\Phi(w_k') - \hat{\nabla}\Phi(w_k')\ \text{ and }\ \varsigma_k'' = \nabla\Phi(w_k'') - \hat{\nabla}\Phi(w_k'').$$

In the last step, we use

$$\nabla\Phi(w_k') - \nabla\Phi(w_k'') = (\mathbf{H} + \mathbf{\Omega}_k)(w_k' - w_k'') = (\mathbf{H} + \mathbf{\Omega}_k)((2-\theta)z_k - (1-\theta)z_{t-1})\ .$$

We thus get the update of z_k in matrix form as follows

$$\begin{aligned}\begin{pmatrix} z_{k+1} \\ z_k \end{pmatrix} &= \begin{pmatrix} (2-\theta)(\mathbf{I} - \eta\mathbf{H}) & -(1-\theta)(\mathbf{I} - \eta\mathbf{H}) \\ \mathbf{I} & 0 \end{pmatrix}\begin{pmatrix} w_k \\ w_{k-1} \end{pmatrix} \\ &\quad + \eta\begin{pmatrix} (2-\theta)\mathbf{\Omega}_k z_k - (1-\theta)\mathbf{\Omega}_k z_{k-1} + \varsigma_k' - \varsigma_k'' \\ 0 \end{pmatrix} \\ &= \mathbf{A}\begin{pmatrix} z_k \\ z_{k-1} \end{pmatrix} - \eta\begin{pmatrix} \omega_k \\ 0 \end{pmatrix} = \mathbf{A}^{k+1}\begin{pmatrix} z_0 \\ z_{-1} \end{pmatrix} - \eta\sum_{i=0}^{k}\mathbf{A}^{k-i}\begin{pmatrix} \omega_i \\ 0 \end{pmatrix}\ ,\end{aligned}$$

where $\omega_k = (2-\theta)\mathbf{\Omega}_k z_k - (1-\theta)\mathbf{\Omega}_k z_{k-1} + \varsigma_k' - \varsigma_k''$. Then we have

$$z_k = \begin{pmatrix} \mathbf{I} & 0 \end{pmatrix}\mathbf{A}^k\begin{pmatrix} z_0 \\ z_0 \end{pmatrix} - \eta\begin{pmatrix} \mathbf{I} & 0 \end{pmatrix}\sum_{i=0}^{k-1}\mathbf{A}^{k-i-1}\begin{pmatrix} \omega_i \\ 0 \end{pmatrix}\ .$$

Assuming that none of the iterations on $(x_0', x_1', \ldots, x_K')$ and $(x_0'', x_1'', \ldots, x_K'')$ trigger the "if condition," then we have

$$\begin{aligned}&\|x_k' - x_0'\|_2 \leq B,\ \|w_k' - x_0'\|_2 \leq 2B,\ \forall k \leq K, \\ &\|x_k'' - x_0''\|_2 \leq B,\ \|w_k'' - x_0''\|_2 \leq 2B,\ \forall k \leq K.\end{aligned} \tag{37}$$

Thus we obtain

$$\begin{aligned}\|\mathbf{\Omega}_k\|_2 &\le \tilde{\rho}\max\left(\|w_k'-x\|_2, \|w_k''-x\|_2\right)\\ &\le \tilde{\rho}\max\left(\|w_k'-x_0'\|_2, \|w_k''-x_0''\|_2\right)+\tilde{\rho}r \le 3\tilde{\rho}B\end{aligned}$$

and

$$\begin{aligned}\|\omega_k\|_2 &\le 6\tilde{\rho}B\left(\|z_k\|_2+\|z_{k-1}\|_2\right)+\|\varsigma_k'-\varsigma_k''\|_2\\ &\le 6\tilde{\rho}B\left(\|z_k\|_2+\|z_{k-1}\|_2\right)+2\sigma,\end{aligned}$$

where we use Lemma 3.3 in the last step. We can show the following inequality for all $k \le K$ by induction:

$$\left\|\eta\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\sum_{i=0}^{k-1}\mathbf{A}^{k-1-i}\begin{pmatrix}\omega_i\\0\end{pmatrix}\right\|_2 \le \frac{1}{2}\left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\mathbf{A}^k\begin{pmatrix}z_0\\z_0\end{pmatrix}\right\|_2.$$

It is easy to check the base case holds for $k=0$. Assume the inequality holds for all steps equal to or less than k. Then we have

$$\|z_k\|_2 \le \frac{3}{2}\left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\mathbf{A}^k\begin{pmatrix}z_0\\z_0\end{pmatrix}\right\|_2 \qquad \text{and} \qquad \|\omega_k\|_2 \le 18\tilde{\rho}B\left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\mathbf{A}^k\begin{pmatrix}z_0\\z_0\end{pmatrix}\right\|_2 + 2\sigma,$$

where we use the monotonicity of $\left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\mathbf{A}^k\begin{pmatrix}z_0\\z_0\end{pmatrix}\right\|_2$ in k (Lemma 38 in Jin et al. (2018)) in the last inequality.

We define

$$\begin{pmatrix}a_k & -b_k\end{pmatrix} = \begin{pmatrix}1 & 0\end{pmatrix}\mathbf{A}_{\min}^k \quad \text{and} \quad \mathbf{A}_{\min} = \begin{pmatrix}(2-\theta)(1-\eta\lambda_{\min}) & -(1-\theta)(1-\eta\lambda_{\min})\\ 1 & 0\end{pmatrix},$$

then

$$\begin{aligned}&\left\|\eta\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\sum_{i=0}^{k}\mathbf{A}^{k-i}\begin{pmatrix}\omega_i\\0\end{pmatrix}\right\|_2\\ &\le \eta\sum_{i=0}^{k}\left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\sum_{i=0}^{k}\mathbf{A}^{k-i}\begin{pmatrix}\mathbf{I}\\0\end{pmatrix}\right\|_2\|\omega_i\|_2\\ &\le \eta\sum_{i=0}^{k}\left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\sum_{i=0}^{k}\mathbf{A}^{k-i}\begin{pmatrix}\mathbf{I}\\0\end{pmatrix}\right\|_2\left(18\tilde{\rho}B\left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\mathbf{A}^i\begin{pmatrix}z_0\\z_0\end{pmatrix}\right\|_2+2\sigma\right)\\ &\overset{(a)}{=} \eta\sum_{i=0}^{k}|a_{k-i}|\,(\,18\tilde{\rho}Br_0|a_i-b_i|+2\sigma)\\ &\overset{(b)}{\le} \eta\sum_{i=0}^{k}|a_{k-i}|\,(\,20\tilde{\rho}Br_0|a_i-b_i|)\\ &\overset{(c)}{\le} 20\tilde{\rho}B\eta\sum_{i=0}^{k}\left(\frac{2}{\theta}+k+1\right)|a_{k+1}-b_{k+1}|r_0\\ &\le 20\tilde{\rho}B\eta K\left(\frac{2}{\theta}+K\right)\left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\mathbf{A}^{k+1}\begin{pmatrix}z_0\\z_0\end{pmatrix}\right\|_2,\end{aligned}$$

where the step $\overset{(a)}{=}$ uses the fact that $z_0 = r_0 e_1$ is along the minimum eigenvector direction of $\mathbf{H}$; the step $\overset{b}{\le}$ is based on the fact that $\sigma \le \tilde{\rho}Br_0|a_i-b_i|$; the step $\overset{c}{\le}$ uses Lemma 36 in (Jin et al., 2018). From Lemma 38 in Jin et al. (2018), we have

$$|a_i-b_i| \ge \frac{\theta}{2}\left(1+\frac{\theta}{2}\right)^i \ge \frac{\theta}{2},$$

and thus $\tilde{\rho}Br_0|a_i - b_i| \geq \dfrac{\tilde{\rho}B\zeta r\theta}{2\sqrt{d_x}} \geq \sigma$. From the parameter settings, we have

$$20\tilde{\rho}B\eta K\left(\frac{2}{\theta} + K\right) \leq \frac{1}{2}.$$

Therefore, we complete the induction, which yields

$$\begin{aligned}
\|z_K\|_2 &\geq \left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\mathbf{A}^K\begin{pmatrix}z_0\\ z_0\end{pmatrix}\right\|_2 - \left\|\eta\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\sum_{i=0}^{K-1}\mathbf{A}^{K-i-1}\begin{pmatrix}\omega_i\\ 0\end{pmatrix}\right\|_2 \\
&\geq \frac{1}{2}\left\|\begin{pmatrix}\mathbf{I} & 0\end{pmatrix}\mathbf{A}^K\begin{pmatrix}z_0\\ z_0\end{pmatrix}\right\|_2 = \frac{r_0}{2}|a_K - b_K| \\
&\geq \frac{\theta r_0}{4}\left(1 + \frac{\theta}{2}\right)^K \geq 5B,
\end{aligned}$$

where we use Lemma 38 in (Jin et al., 2018) and $\eta\lambda_{\min} \leq -\theta^2$ in the third inequality and the last step comes from $K = \frac{2}{\theta}\log(\frac{20B}{\theta r_0})$. However, from equation (37) we obtain:

$$\|z_K\|_2 \leq \|x'_K - x'_0\|_2 + \|x''_K - x''_0\|_2 + \|x'_0 - x''_0\|_2 \leq 2B + 2r \leq 4B,$$

which leads to a contradiction. Thus we conclude that at least one of the iteration triggers the "if condition" and we finish the proof. □

Having established the necessary groundwork, we are now prepared to present the proof of Theorem 4.1.

Proof. From Lemma C.1, we know that Algorithm 3 will terminate in at most $\mathcal{O}\left(\Delta\sqrt{\tilde{\rho}}\chi^5\epsilon^{-3/2}\right)$ epochs. Since each epoch needs at most $K = \mathcal{O}\left(\chi\left(\tilde{L}^2/(\epsilon\tilde{\rho})\right)^{1/4}\right)$ gradient evaluations, the total number of gradient evaluations must be less than $\mathcal{O}\left(\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\chi^6\epsilon^{-1.75}\right)$.
Now we consider the last epoch. Following a similar methodology employed in the proof of Theorem 3.4, we also have

$$\|\nabla\Phi(\hat{w})\|_2 \leq \frac{2\sqrt{2}B}{\eta K^2} + \frac{2\theta B}{\eta K} + 4\tilde{\rho}B^2 + \sigma \leq \frac{\epsilon}{\chi^3} + \epsilon^2 \leq \epsilon\ .$$

If $\lambda_{\min}(\nabla^2\Phi(x_{t,\mathcal{K}})) \geq -\sqrt{\epsilon\tilde{\rho}}$, then from the perturbation theory of eigenvalues of Bhatia (1997), we have

$$\begin{aligned}
|\lambda_j(\nabla^2\Phi(\hat{w}_{t+1})) - \lambda_j(\nabla^2\Phi(x_{t,\mathcal{K}}))| &\leq \left\|\nabla^2\Phi(\hat{w}_{t+1}) - \nabla^2\Phi(x_{t,\mathcal{K}})\right\|_2 \\
&\leq \tilde{\rho}\left\|\hat{w}_{t+1} - x_{t,\mathcal{K}}\right\|_2 \\
&\leq \tilde{\rho}\left\|\hat{w}_{t+1} - x_{t+1,0}\right\|_2 + \tilde{\rho}r \\
&\leq 3\tilde{\rho}B
\end{aligned}$$

for any j, where we use $\left\|\hat{w}_{t+1} - x_{t+1,0}\right\|_2 \leq \frac{1}{K_0+1}\sum_{k=0}^{K_0}\left\|w_{t+1,k} - x_{t+1,0}\right\|_2 \leq 2B$ in the last inequality. Then we have

$$\begin{aligned}
\lambda_j(\nabla^2\Phi(\hat{w}_{t+1})) &\geq \lambda_j(\nabla^2\Phi(x_{t,\mathcal{K}})) - |\lambda_j(\nabla^2\Phi(\hat{w}_{t+1})) - \lambda_j(\nabla^2\Phi(x_{t,\mathcal{K}}))| \\
&\geq -\sqrt{\epsilon\tilde{\rho}} - 3\tilde{\rho}B \geq -1.011\sqrt{\epsilon\tilde{\rho}}.
\end{aligned}$$

Now we consider $\lambda_{\min}(\nabla^2\Phi(x_{t,\mathcal{K}})) < -\sqrt{\epsilon\tilde{\rho}}$. Define the stuck region in $\mathbb{B}(r)$ centered at $x_{t,\mathcal{K}}$ to be the set of points starting from which the "if condition" does not trigger in K iterations, that is, the algorithm terminates and outputs a saddle point. From Lemma C.2, we know that the length along the minimum eigen-direction of $\nabla^2\Phi(x_{t,\mathcal{K}})$ is less than r_0. Therefore, the probability of the starting point $x_{t+1,0} = x_{t,\mathcal{K}} + \xi_t$ located in the stuck region is less than

$$\frac{r_0 V_{d-1}(r)}{V_d(r)} \leq \frac{r_0\sqrt{d}}{r} \leq \zeta,$$

where we let $r_0 = \frac{\zeta r}{\sqrt{d}}$. Thus, the output $\hat{w}$ satisfies $\lambda_{\min}(\nabla^2\Phi(\hat{w}) \geq -1.011\sqrt{\epsilon\tilde{\rho}}$ with probability at least $1 - \zeta$. This completes the proof of Theorem 4.1. □

C.2 Proof of Proposition 4.2

The proof of Proposition 4.2 is similar to that of Proposition 3.5. We provide the proof for Proposition 4.2 as follows.

Proof. We first consider the iterations of CG in Algorithm 3 in one epoch. We choose $T'_{t,k}$ as

$$T'_{t,k} = \begin{cases} \left\lceil \frac{\sqrt{\kappa}+1}{2} \log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\|v_{0,-1}\|_2 + \frac{M}{\mu}\right)\right)\right\rceil, & k = 0, \\ \left\lceil \frac{\sqrt{\kappa}+1}{2} \log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\frac{\sigma}{2\ell} + \frac{2M}{\mu}\right)\right)\right\rceil, & k \geq 1. \end{cases} \tag{38}$$

Following along the lines of the proof in Section B.2 we see that equation (7) in Condition 3.1 holds.

The total iterate count of CG when running `PRAHGD` in Algorithm 3 in one epoch satisfies

$$\begin{aligned} \sum_{k=0}^{\mathcal{K}-1} T'_k &\leq \mathcal{K} + \frac{\sqrt{\kappa}+1}{2}\left(\frac{2T'_0}{\sqrt{\kappa}+1} + \sum_{k=1}^{\mathcal{K}-1} \log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\frac{\sigma}{2\ell} + \frac{2M}{\mu}\right)\right)\right) \\ &= \mathcal{K} + \frac{\sqrt{\kappa}+1}{2}\left(\frac{2T'_0}{\sqrt{\kappa}+1} + (\mathcal{K}-1)\log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\frac{\sigma}{2\ell} + \frac{2M}{\mu}\right)\right)\right) \\ &= \mathcal{K} + \frac{\sqrt{\kappa}+1}{2}\mathcal{K}\left(\frac{1}{\mathcal{K}}\log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\|v_{0,-1}\|_2 + \frac{M}{\mu}\right)\right) + \left(1-\frac{1}{\mathcal{K}}\right)\log\left(\frac{4\ell\sqrt{\kappa}}{\sigma}\left(\frac{\sigma}{2\ell} + \frac{2M}{\mu}\right)\right)\right) . \end{aligned}$$

Now we consider the iterations of AGD `PRAHGD` in Algorithm 3 in one epoch.

We first show the following lemma.

Lemma C.3. *Consider the setting of Theorem 4.1, and we run* `PRAHGD` *in Algorithm 3, then we have*

$$\|y^*(w_{t,-1})\|_2 \leq \tilde{C}$$

for any $t > 0$, where $\tilde{C} = \|y^*(x_{0,0})\|_2 + (2B + B^2 + \eta\sigma + \eta C)\kappa\Delta\sqrt{\bar{\rho}}\epsilon^{-3/2}$.

Then we choose $T_{t,k}$ as

$$T_{t,k} = \begin{cases} \left\lceil 2\sqrt{\kappa}\log\left(\frac{2\tilde{L}\sqrt{\kappa+1}}{\sigma}\tilde{C}\right)\right\rceil, & k = -1 \\ \left\lceil 2\sqrt{\kappa}\log\left(\frac{2\tilde{L}\sqrt{\kappa+1}}{\sigma}\left(\frac{\sigma}{2\tilde{L}} + 2\kappa B\right)\right)\right\rceil, & k \geq 0 \end{cases} \tag{39}$$

We will use induction to show that Lemma C.3 as well as equation (6) in Condition 3.1 will hold.

For $t = 0$, Lemma C.3 hold trivially. Then we use induction with respect to k to prove that

$$\|y_{t,k} - y^*(w_{t,k})\|_2 \leq \frac{\sigma}{2\tilde{L}}$$

holds for any $k \geq -1$. For $k = -1$, Lemma 2.1 directly implies

$$\|y_{t,-1} - y^*(w_{t,-1})\|_2 \leq \frac{\left\|y^*(w_{t,-1})\right\|_2}{\tilde{C}} \cdot \frac{\sigma}{2\tilde{L}} \leq \frac{\sigma}{2\tilde{L}},$$

where the second inequality is based on Lemma C.3. Suppose it holds that $\|y_{t,k-1} - y^*(w_{t,k-1})\|_2 \leq \frac{\sigma}{2\tilde{L}}$ for any $k \leq k' - 1$, then we have

$$\begin{aligned} &\|y_{t,k'} - y^*(w_{t,k'})\|_2 \\ &\quad\leq \sqrt{1+\kappa}\left(1 - \frac{1}{\sqrt{\kappa}}\right)^{T_{t,k'}/2} \|y_{t,k'-1} - y^*(w_{t,k'})\|_2 \\ &\quad\leq \sqrt{1+\kappa}\left(1 - \frac{1}{\sqrt{\kappa}}\right)^{T_{t,k'}/2} (\|y_{t,k'-1} - y^*(w_{t,k'-1})\|_2 + \|y^*(w_{t,k'-1}) - y^*(w_{t,k'})\|_2) \end{aligned}$$

$$
\begin{aligned}
&\leq \sqrt{1+\kappa}\left(1-\frac{1}{\sqrt{\kappa}}\right)^{T_{t,k'}/2}\left(\frac{\sigma}{2\tilde{L}}+\kappa\left\|w_{t,k'-1}-w_{t,k'}\right\|_2\right)\\
&\leq \sqrt{1+\kappa}\left(1-\frac{1}{\sqrt{\kappa}}\right)^{T_{t,k'}/2}\left(\frac{\sigma}{2\tilde{L}}+2\kappa B\right)\\
&\leq \frac{\sigma}{2\tilde{L}}\ ,
\end{aligned}
$$

where the first inequality is based on Lemma 2.1, the second one uses the triangle inequality, the third one is based on the induction hypothesis and Lemma 2.5, the fourth one uses equation (12), and the last step use the definition of $T_{t,k}$. Therefore, equation (6) in Condition 3.1 holds.

Suppose Lemma C.3 and equation (6) in Condition 3.1 hold for any $t \leq t'-1$, then we have shown that when we choose $T'_{t,k}$ as defined in equation (38), then equation (7) in Condition 3.1 holds. Thus, from Lemma 3.3 we obtain that:

$$
\|\nabla\Phi(w_{t,k})-\hat{\nabla}\Phi(w_{t,k})\|_2 \leq \sigma\ . \tag{40}
$$

For any epoch $t \leq t'-1$, we have

$$
\begin{aligned}
&\left\|x_{t,\mathcal{K}}-x_{t,0}\right\|_2\\
&\quad=\left\|x_{t,\mathcal{K}}-x_{t,\mathcal{K}-1}+x_{t,\mathcal{K}-1}-x_{t,0}\right\|_2\\
&\quad=\left\|(1-\theta)(x_{t,\mathcal{K}-1}-x_{t,\mathcal{K}-2})-\eta\hat{\nabla}\Phi(w_{t,\mathcal{K}-1})+x_{t,\mathcal{K}-1}-x_{t,0}\right\|_2\\
&\quad\leq\left\|x_{t,\mathcal{K}-1}-x_{t,\mathcal{K}-2}\right\|_2+\left\|x_{t,\mathcal{K}-1}-x_{t,0}\right\|_2+\eta\left\|\hat{\nabla}\Phi(w_{t,\mathcal{K}-1)}\right\|_2\\
&\quad\leq 2B+\eta\left\|\hat{\nabla}\Phi(w_{t,\mathcal{K}-1})-\nabla\Phi(w_{t,\mathcal{K}-1})+\nabla\Phi(w_{t,\mathcal{K}-1})\right\|_2\\
&\quad\leq 2B+\eta\left\|\hat{\nabla}\Phi(w_{t,\mathcal{K}-1})-\nabla\Phi(w_{t,\mathcal{K}-1})\right\|_2+\eta\left\|\nabla\Phi(w_{t,\mathcal{K}-1})\right\|_2\\
&\quad\leq 2B+\eta\sigma+\eta\left\|\nabla\Phi(w_{t,\mathcal{K}-1})\right\|_2\\
&\quad\leq 2B+\eta(\sigma+C)
\end{aligned}
\tag{41}
$$

for some constant C. Here we use the triangle inequality in the first inequality, equation (10) in the second one, the triangle inequality again in the third one, equation (40) in the fourth one and equation (33) in the last one.

Then for the t'-th epoch, we have

$$
\begin{aligned}
&\left\|y^*(w_{t',-1})-y^*(x_{0,0})\right\|_2\\
&\quad\leq\kappa\left\|w_{t',-1}-x_{0,0}\right\|_2\\
&\quad=\kappa\left\|x_{t',0}-x_{0,0}\right\|_2\\
&\quad=\kappa\left\|x_{t'-1,\mathcal{K}}-x_{0,0}\right\|_2\\
&\quad\leq\kappa(\left\|x_{t'-1,0}-x_{0,0}\right\|_2+\left\|x_{t'-1,\mathcal{K}}-x_{t'-1,0}\right\|_2+r)\\
&\quad\leq\kappa(\left\|x_{t'-1,0}-x_{1,0}\right\|_2+(2B+B^2+\eta\sigma+\eta C))\\
&\quad\leq(2B+B^2+\eta\sigma+\eta C)\kappa t\ ,
\end{aligned}
$$

where the first inequality is based on the Lipschitz continuity of $y^*(x)$ shown in Lemma 2.5, the second one uses the triangle inequality, the third one is based on equation (41), and the last one uses induction. Then we have

$$
\left\|y^*(w_{t',-1})\right\|_2 \leq \left\|y^*(x_{0,0})\right\|_2+B\kappa t' \leq \left\|y^*(x_{0,0})\right\|_2+\frac{(2B+B^2+\eta\sigma+\eta C)\kappa\Delta\sqrt{\bar{\rho}}}{\epsilon^{3/2}},
$$

where we use Lemma C.1 in the last inequality.

Similarly with the case $t=0$, we use induction with respect to k which allows us to prove that equation (6) in Condition 3.1 holds. This also completes the proof for Lemma C.3.

The total number of gradient calls from AGD in Algorithm 3 in one epoch satisfies

$$
\sum_{k=-1}^{\mathcal{K}-1} T_{t,k} \leq 2\sqrt{\kappa}\left(\frac{T_{t,-1}}{2\sqrt{\kappa}}+\sum_{k=0}^{\mathcal{K}-1}\log\left(\sqrt{\kappa+1}+\frac{4\tilde{L}\kappa\sqrt{\kappa+1}B}{\sigma}\right)\right)+\mathcal{K}+1
$$

$$= 2\sqrt{\kappa}\left(\frac{T_{t,-1}}{2\sqrt{\kappa}} + \mathcal{K}\log\left(\sqrt{\kappa+1} + \frac{4\tilde{L}\kappa\sqrt{\kappa+1}B}{\sigma}\right)\right) + \mathcal{K} + 1$$
$$= 2\sqrt{\kappa}\mathcal{K}\left(\frac{1}{\mathcal{K}}\log\left(\frac{2\tilde{L}\sqrt{\kappa+1}}{\sigma}\tilde{C}\right) + \log\left(\sqrt{\kappa+1} + \frac{4\tilde{L}\kappa\sqrt{\kappa+1}B}{\sigma}\right)\right) + \mathcal{K} + 1.$$

This finishes our proof of Proposition 4.2. □

C.3 Proof of Corollary 4.3

Proof. From Theorem 4.1, we have that PRAHGD in Algorithm 3 can find an $(\epsilon, \sqrt{\tilde{\rho}\epsilon})$ SOSP within at most $\mathcal{O}\left(\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\chi^6\epsilon^{-7/4}\right)$ iterations in the outer loop. Thus we have

$$Gc(f,\epsilon) = \mathcal{O}\left(\frac{\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\chi^6}{\epsilon^{7/4}}\right) \qquad \text{and} \qquad JV(g,\epsilon) = \mathcal{O}\left(\frac{\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\chi^6}{\epsilon^{7/4}}\right).$$

Omitting polylogarithmic factors and plugging in $\tilde{L} = \mathcal{O}(\kappa^3)$ and $\tilde{\rho} = \mathcal{O}(\kappa^5)$, we have

$$Gc(f,\epsilon) = \tilde{\mathcal{O}}\left(\kappa^{11/4}\epsilon^{-7/4}\right) \qquad \text{and} \qquad JV(g,\epsilon) = \tilde{\mathcal{O}}\left(\kappa^{11/4}\epsilon^{-7/4}\right).$$

Lemma C.1 shows that PRAHGD in Algorithm 3 will terminate in at most $\mathcal{O}\left(\frac{\Delta\sqrt{\tilde{\rho}}\chi^5}{\epsilon^{3/2}}\right)$ epochs. From Proposition 4.2 we can obtain that for each epoch t, we have the following bounds for the inner loops:

$$\sum_{k=-1}^{\mathcal{K}-1} T_{t,k} \le \mathcal{O}\left(\kappa^{1/2}\mathcal{K}\log(1/\epsilon)\right) \qquad \text{and} \qquad \sum_{k=0}^{\mathcal{K}-1} T'_{t,k} \le \mathcal{O}\left(\kappa^{1/2}\mathcal{K}\log(1/\epsilon)\right).$$

Thus we have

$$Gc(g,\epsilon) = \mathcal{O}\left(\frac{\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\kappa^{1/2}\chi^6\log(1/\epsilon)}{\epsilon^{7/4}}\right) \text{ and } HV(g,\epsilon) = \mathcal{O}\left(\frac{\Delta\tilde{L}^{1/2}\tilde{\rho}^{1/4}\kappa^{1/2}\chi^6\log(1/\epsilon)}{\epsilon^{7/4}}\right),$$

where we use $\mathcal{K} \le K = \mathcal{O}\big(\chi\big(\tilde{L}^2/(\epsilon\tilde{\rho})\big)^{1/4}\big)$. Omitting polylogarithmic factor and plugging in $\tilde{L} = \mathcal{O}(\kappa^3)$ and $\tilde{\rho} = \mathcal{O}(\kappa^5)$, we have

$$Gc(g,\epsilon) = \tilde{\mathcal{O}}\left(\kappa^{13/4}\epsilon^{-7/4}\right) \qquad \text{and} \qquad HV(g,\epsilon) = \tilde{\mathcal{O}}\left(\kappa^{13/4}\epsilon^{-7/4}\right).$$

This completes our proof of Corollary 4.3. □

D Algorithm and Proofs in Section 5

We first show more details for PRAGDA in Algorithm 4.

Algorithm 4 PRAGDA

Input: initial vector $x_{0,0}$; step-size $\eta > 0$; momentum param. $\theta \in (0,1)$; params. $\alpha > 0, \beta \in (0,1), \{T_{t,k}\}$ of AGD; iteration threshold $K \geq 1$; param. B for triggering restarting; perturbation radius $r > 0$
$k \leftarrow 0,\ t \leftarrow 0,\ x_{0,-1} \leftarrow x_{0,0}$
$y_{0,-1} \leftarrow \mathrm{AGD}(-\bar{f}(x_{0,-1}, \cdot), 0, T_{0,-1}, \alpha, \beta)$
while $k < K$
  $w_{t,k} \leftarrow x_{t,k} + (1-\theta)(x_{t,k} - x_{t,k-1})$
  $y_{t,k} \leftarrow \mathrm{AGD}(-\bar{f}(w_{t,k}, \cdot), y_{t,k-1}, T_{t,k}, \alpha, \beta)$
  $x_{t,k+1} \leftarrow w_{t,k} - \eta \nabla_x \bar{f}(w_{t,k}, y_{t,k})$
  $k \leftarrow k+1$
  if $k \sum_{i=0}^{k-1} \|x_{t,i+1} - x_{t,i}\|^2 > B^2$
    $x_{t+1,0} \leftarrow x_{t,k} + \xi_{t,k},\ \xi_{t,k} \sim \mathrm{Unif}(\mathbb{B}(r))$
    $x_{t+1,-1} \leftarrow x_{t+1,0}$
    $k \leftarrow 0,\ t \leftarrow t+1$
    $y_{t,-1} \leftarrow \mathrm{AGD}(-\bar{f}(x_{t,-1}, \cdot), 0, T_{t,-1}, \alpha, \beta)$
  end if
end while
$K_0 \leftarrow \arg\min_{\lfloor \frac{K}{2} \rfloor \leq k \leq K-1} \|x_{t,k+1} - x_{t,k}\|_2$
Output: $\hat{w} \leftarrow \frac{1}{K_0+1} \sum_{k=0}^{K_0} w_{t,k}$

Now we provide the proof of Theorem 5.2.

Proof. Lemma 5.1 shows that in minimax problem settings, $\tilde{L} = (\kappa+1)\ell$ and $\tilde{\rho} = 4\sqrt{2}\kappa^3\rho$. Recall that our PRAGDA evolves directly from PRAHGD—removing the CG step in PRAHGD because we do not need to compute the Hessian-vector products when solving the minmax problem. Therefore, we can straightforwardly apply the theoretical results for PRAHGD.

Applying Theorem 4.1, we have that Algorithm 4 can find an $\big(\epsilon, \mathcal{O}(\kappa^{1.5}\sqrt{\epsilon}\,)\big)$-SOSP.

Now we bound the number of gradient oracle calls. From Lemma C.1, we know that Algorithm 4 will terminate in at most $\mathcal{O}\big(\Delta\sqrt{\tilde{\rho}}\chi^5\epsilon^{-3/2}\big)$ epochs. Proposition 4.2 shows that, for each t, the total iteration count for an AGD step satisfies:

$$\sum_{k=-1}^{\mathcal{K}-1} T_{t,k} \leq \mathcal{O}(\kappa^{1/2}\mathcal{K}\log(1/\epsilon)) \ .$$

Recalling that $\mathcal{K} \leq K = \mathcal{O}\left(\chi\big(\tilde{L}^2/(\epsilon\tilde{\rho})\big)^{1/4}\right)$, we have that the total number of gradient oracle calls is at most:

$$\mathcal{O}\left(\frac{\Delta\tilde{\rho}^{1/4}\tilde{L}^{1/2}\kappa^{1/2}\chi^6\log(1/\epsilon)}{\epsilon^{7/4}}\right) \ .$$

Hiding polylogarithmic factor and plugging in $\tilde{L}$ and $\tilde{\rho}$, we have that the total number of gradient oracle calls is at most $\tilde{\mathcal{O}}(\kappa^{7/4}\epsilon^{-7/4})$. □

E Discussions on Comparisons with "Fully First-Order Methods"

In this section, we draw connections of our proposed algorithmic framework with the recently proposed *fully first-order methods* for bilevel optimization (Kwon et al., 2023; Chen et al., 2023). Kwon et al. (2023) considers the first-order approximation for bilevel optimization problem (1a)–(1b) where they introduce the auxiliary function

as follows:

$$\mathcal{L}_\lambda(x,y) \triangleq f(x,y) + \lambda\left(g(x,y) - \min_{z\in\mathbb{R}^{d_y}} g(x,z)\right), \tag{42}$$

where the regularization parameter $\lambda > 0$. Under Assumptions 2.3(i)–(iv), taking $\lambda \geq 2\kappa = \frac{2\ell}{\mu}$ leads to $\mathcal{L}_\lambda(x,y)$ being strongly convex in y for any given x, which implies that the function

$$\mathcal{L}_\lambda^*(x) \triangleq \min_{y\in\mathbb{R}^{d_y}} \mathcal{L}_\lambda(x,y) \tag{43}$$

is smooth (Danskin, 2012).

By setting λ appropriately, the approximate first-order and second-order stationary points of the objective $\Phi(x) \triangleq f(x, y^*(x))$ in bilevel problem (1a)–(1b) are sufficiently close to the corresponding stationary points. This implies we can address the bilevel problem by considering the minimization problem

$$\min_{x\in\mathbb{R}^{d_x}} \left\{\mathcal{L}_\lambda^*(x) \triangleq \min_{y\in\mathbb{R}^{d_y}} \mathcal{L}_\lambda(x,y)\right\}. \tag{44}$$

The expression of $\mathcal{L}_\lambda(x,y)$ shown in (42) indicates we can solve problem (44) by only accessing the first-order oracles of $f(x,y)$ and $g(x,y)$. Based on this idea, Kwon et al. (2023) proposed a fully first-order method for finding ϵ-first-order stationary points of $\Phi(x)$ with a first-order oracle complexity of ϵ^{-3}.

Very recently and concurrent to our work, Chen et al. (2023) revisits the fully first-order methods Kwon et al. (2023) and improves the first-order oracle complexity to $\tilde{\mathcal{O}}(\kappa^4\epsilon^{-2})$. The key observation is that the Lipschitz continuous constant of $\mathcal{L}_\lambda^*(x)$ can be set to be *not* dependent on ϵ. By further assuming that $g(x,y)$ admits Lipschitz continuous third-order derivatives (Assumption 2.3(v)), Chen et al. (2023) also provided a perturbed first-order method to find $(\epsilon, \mathcal{O}(\kappa^{2.5}\sqrt{\epsilon}\,))$-second-order stationary points of $\Phi(x)$ within $\tilde{\mathcal{O}}(\kappa^4\epsilon^{-2})$ first-order oracle complexity.

In this section, we illustrate that our acceleration framework can be effectively incorporated into the idea of fully first-order methods, improving the dependency on ϵ from ϵ^{-2} to $\epsilon^{-1.75}$. We first present some properties of function $\mathcal{L}_\lambda^*(x)$ and its connection to function $\Phi(x)$ in the following lemma (Chen et al., 2023).

Lemma E.1. *Suppose Assumption 2.3(i)–(iv) hold and set $\lambda \geq 2\kappa$, then*

(i) $|\mathcal{L}_\lambda^*(x) - \Phi(x)| \leq \mathcal{O}(\kappa^2/\lambda)$ *for any* $x \in \mathbb{R}^{d_x}$;

(ii) $\|\nabla\mathcal{L}_\lambda^*(x) - \nabla\Phi(x)\|_2 \leq \mathcal{O}(\kappa^3/\lambda)$ *for any* $x \in \mathbb{R}^{d_x}$;

(iii) $\mathcal{L}_\lambda^*(x)$ *is* L_λ*-gradient Lipschitz, where* $L_\lambda \leq \mathcal{O}(\kappa^3)$.

If we further suppose Assumption 2.3(v) holds, then

(i) $\left\|\nabla^2\mathcal{L}_\lambda^*(x) - \nabla^2\Phi(x)\right\|_2 \leq \mathcal{O}(\kappa^6/\lambda)$ *for any* $x \in \mathbb{R}^{d_x}$;

(ii) $\mathcal{L}_\lambda^*(x)$ *is* ρ_λ*-Hessian Lipschitz, where* $\rho_\lambda \leq \mathcal{O}(\kappa^5)$.

The detailed expression for the upper bounds of $\|\nabla\mathcal{L}_\lambda^*(x) - \nabla\Phi(x)\|_2$, L_λ, $|\mathcal{L}_\lambda^*(x) - \Phi(x)|$, $\left\|\nabla^2\mathcal{L}_\lambda^*(x) - \nabla^2\Phi(x)\right\|_2$ and ρ_λ can be found in Appendix E.1.

We proposed our (perturbed) restarted accelerated *Fully First-order methods for Bilevel Approximation* ($\mathrm{F^2BA}$) in Algorithm 5. The theoretical guarantees of this algorithm is presented as follows:

Theorem E.2 (finding ϵ-FOSP)**.** *Suppose Assumptions 2.3 holds. We denote* $\Delta = \Phi(x_{\text{int}}) - \min_{x\in\mathbb{R}^{d_x}} \Phi(x)$ *and* $\kappa' = (\lambda+1)\ell/(\lambda\mu - \ell)$. *Let*

$$\eta = \frac{1}{4L_\lambda}, \quad B = \sqrt{\frac{\epsilon}{\rho_\lambda}}, \quad \theta = 4(\rho_\lambda\epsilon\eta^2)^{1/4}, \quad K = \frac{1}{\theta}, \quad \alpha = \frac{1}{\ell}, \quad \beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1},$$

$$\lambda = \Theta\left(\max\{\kappa^2/\Delta,\ \kappa^3/\epsilon\}\right), \quad \alpha' = \frac{1}{(\lambda+1)\ell}, \quad \beta' = \frac{\sqrt{\kappa'}-1}{\sqrt{\kappa'}+1}, \quad \sigma = \epsilon^2$$

and assume that $\mathcal{O}(\epsilon) \leq L_\lambda^2/\rho_\lambda$. *Then our* `RAF²BA` *(Algorithm 5) can find an* $\mathcal{O}(\epsilon)$*-first-order stationary point of* $\Phi(x)$. *Additionally, the oracle complexities satisfy* $Gc(f,\epsilon) = Gc(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$.

Algorithm 5 (Perturbed) Restarted Accelerated F^{2}BA, `(P)RAF$^2$BA`

Input: initial vector $x_{0,0}$; step-size $\eta > 0$; momentum parameter $\theta \in (0,1)$; parameters $\alpha, \alpha' > 0, \beta, \beta' \in (0,1), \{T_{t,k}\}, \{T'_{t,k}\}$ of AGD; iteration threshold $K \geq 1$; parameter B for triggering restarting; perturbation radius $r > 0$; option `Perturbation` $\in \{0,1\}$

$k \leftarrow 0,\ t \leftarrow 0,\ x_{0,-1} \leftarrow x_{0,0}$

$y_{0,-1} \leftarrow \mathrm{AGD}(f(x_{0,-1}, \cdot) + \lambda g(x_{0,-1}, \cdot), 0, T'_{0,-1}, \alpha', \beta')$

$z_{0,-1} \leftarrow \mathrm{AGD}(g(x_{0,-1}, \cdot), 0, T_{0,-1}, \alpha, \beta)$

while $k < K$

  $w_{t,k} \leftarrow x_{t,k} + (1-\theta)(x_{t,k} - x_{t,k-1})$

  $z_{t,k} \leftarrow \mathrm{AGD}(g(w_{t,k}, \cdot), z_{t,k-1}, T_{t,k}, \alpha, \beta)$

  $y_{t,k} \leftarrow \mathrm{AGD}(f(w_{t,k}, \cdot) + \lambda g(w_{t,k}, \cdot), y_{t,k-1}, T'_{t,k}, \alpha', \beta')$

  $u_{t,k} \leftarrow \nabla_x f(w_{t,k}, y_{t,k}) + \lambda(\nabla_x g(w_{t,k}, y_{t,k}) - \nabla_x g(w_{t,k}, z_{t,k}))$

  $x_{t,k+1} \leftarrow w_{t,k} - \eta u_{t,k}$

  $k \leftarrow k+1$

  if $k \sum_{i=0}^{k-1} \|x_{t,i+1} - x_{t,i}\|^2 > B^2$

    if `Perturbation` $= 0$

      $x_{t+1,0} \leftarrow x_{t,k}$

    else:

      $x_{t+1,0} \leftarrow x_{t,k} + \xi_{t,k}$ with $\xi_{t,k} \sim \mathrm{Unif}(\mathbb{B}(r))$

    end if

    $x_{t+1,-1} \leftarrow x_{t+1,0}$

    $y_{t+1,-1} \leftarrow \mathrm{AGD}(f(x_{t+1,-1}, \cdot) + \lambda g(x_{t+1,-1}, \cdot), 0, T'_{t+1,-1}, \alpha', \beta')$

    $z_{t+1,-1} \leftarrow \mathrm{AGD}(g(x_{t+1,-1}, \cdot), 0, T_{t+1,-1}, \alpha, \beta)$

    $k \leftarrow 0,\ t \leftarrow t+1$

  end if

end while

$K_0 \leftarrow \arg\min_{\lfloor \frac{K}{2} \rfloor \leq k \leq K-1} \|x_{t,k+1} - x_{t,k}\|_2$

Output: $\hat{w} \leftarrow \frac{1}{K_0+1} \sum_{k=0}^{K_0} w_{t,k}$

Theorem E.3 (finding $(\epsilon, O(\kappa^{2.5}\sqrt{\epsilon}))$-SOSP)**.** *Suppose Assumption 2.3 holds. We denote* $\Delta = \Phi(x_{\mathrm{int}}) - \min_{x \in \mathbb{R}^{d_x}} \Phi(x)$ *and* $\kappa' = (\lambda+1)\ell/(\lambda\mu - \ell)$*. Let*

$$\chi = \mathcal{O}\left(\log \frac{d_x}{\zeta\epsilon}\right), \quad \eta = \frac{1}{4L_\lambda}, \quad K = \frac{2\chi}{\theta}, \quad B = \frac{1}{288\chi^2}\sqrt{\frac{\epsilon}{\rho_\lambda}}, \quad \theta = \frac{1}{2}(\rho_\lambda \epsilon \eta^2)^{1/4}, \quad \sigma = \min\left\{\frac{\rho_\lambda B \zeta r \theta}{2\sqrt{d_x}}, \epsilon^2\right\},$$

$$\alpha = \frac{1}{\ell}, \quad \beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}, \quad \alpha' = \frac{1}{(\lambda+1)\ell}, \quad \beta' = \frac{\sqrt{\kappa'}-1}{\sqrt{\kappa'}+1}, \quad \lambda = \Theta\left(\max\{\kappa^2/\Delta,\ \kappa^3/\epsilon,\ \kappa^6/\sqrt{\epsilon}\}\right),$$

$$r = \min\left\{\frac{L_\lambda B^2}{4C}, \frac{B+B^2}{\sqrt{2}}, \frac{\theta B}{20K}, \sqrt{\frac{\theta B^2}{2K}}\right\}$$

for some positive constant C *and assume that* $\epsilon \leq L_\lambda^2/\rho_\lambda$*. Then our* `PRAF$^2$BA` *(Algorithm 5) can find an* $(\mathcal{O}(\epsilon), O(\kappa^{2.5}\sqrt{\epsilon}))$*-second-order stationary point of* $\Phi(x)$ *with probability at least* $1-\zeta$*. Additionally, the oracle complexities satisfy* $Gc(f,\epsilon) = Gc(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$ *.*

Before ending this section we point out the connection between our (perturbed) *restarted accelerated hyperGradient descent* and the (perturbed) *restarted accelerated fully first-order methods*; that is, when applying to the minimax problem (8), the procedures of Algorithm 5 and Algorithm 4 are *identical* with the appropriate parameters setup. As indicated by Section 5, the minimax problem (8) can be reformulated as the bilevel optimization problem equation (1a)—equation (1b) with $f(x,y) = \bar{f}(x,y)$ and $g(x,y) = -\bar{f}(x,y)$. We emphasize

that by taking $\lambda > 1$, the regularized objective $\mathcal{L}_\lambda^*(x)$ is exactly equal to the objective function $\bar{\Phi}(x)$ in minimax problem (8).[4] Careful examination of the algorithm procedures indicates that applying Algorithm 5 to minimizing $\mathcal{L}_\lambda^*(x)$ with $\alpha = \alpha'$ and $\beta = \beta'$ leads to that the $y_{t,k} = z_{t,k}$ always holds, since the sequences $\{y_{t,k}\}$ and $\{z_{t,k}\}$ correspond to the iterations for problems $\min_{y\in\mathbb{R}^{d_y}} -f(w_{t,k}, y)$ and $\min_{y\in\mathbb{R}^{d_y}} -(\lambda-1)f(w_{t,k}, y)$, respectively. Hence, Lines 7–8 of Algorithm 5 is identical to Line 7 of Algorithm 4 when $\eta = \eta_x$, proving the equivalence. Therefore under this setup, the statement of Theorem 5.2 also holds for Algorithm 5.

In the remains of this section, we provide more details for Lemma E.1, Theorem E.2 and Theorem E.3.

E.1 More details of Lemma E.1

We present the detailed expression of the upper bounds in Lemma E.1 as follows.

Lemma E.4. *(Chen et al., 2023, Sections B and C) Suppose Assumption 2.3(i)-(iv) hold and set $\lambda \geq 2\kappa$, then*

(i) $|\mathcal{L}_\lambda^*(x) - \Phi(x)| \leq D_0/\lambda$ for any $x \in \mathbb{R}^{d_x}$, where

$$D_0 = \left(M + \frac{M\ell}{2\mu}\right)\frac{M}{\mu} = \mathcal{O}(\kappa^2);$$

(ii) $\|\nabla\mathcal{L}_\lambda^*(x) - \nabla\Phi(x)\|_2 \leq D_1/\lambda$, where

$$D_1 = \left(\ell + \frac{2\rho\ell + M\rho}{2\mu} + \frac{M\rho\ell}{2\mu^2}\right)\frac{M}{\mu} = \mathcal{O}(\kappa^3); \tag{45}$$

(iii) $\mathcal{L}_\lambda^*(x)$ is L_λ-Lipschitz, where

$$L_\lambda = \ell + \frac{5\ell^2 + M\rho}{\mu} + \frac{2M\ell\rho + 2\ell^3}{\mu^2} + \frac{2M\ell^2\rho}{\mu^3} = \mathcal{O}(\kappa^3).$$

If we further suppose Assumption 2.3(v) holds, then

(i) $\left\|\nabla^2\mathcal{L}_\lambda^*(x) - \nabla^2\Phi(x)\right\|_2 \leq D_2/\lambda$ for any $x \in \mathbb{R}^{d_x}$, where

$$D_2 = 2\ell\left(1 + \frac{2\ell}{\mu}\right)^2\left(\frac{\ell}{\mu} + \frac{M\rho}{\mu^2}\right)^2 + \left(1 + \frac{\ell}{\mu}\right)^2\left(\frac{M\rho}{\mu} + \frac{M\ell\rho}{\mu^2} + \frac{M^2\nu}{2\mu^2} + \frac{M^2\rho^2}{2\mu^3}\right) = \mathcal{O}(\kappa^6);$$

(ii) $\mathcal{L}_\lambda^*(x)$ is ρ_λ-Hessian Lipschitz, where

$$\begin{aligned}\rho_\lambda = {} & \left(1 + \frac{4\ell}{\mu}\right)^2\left(3\rho + \frac{2\ell\rho}{\mu}\right) + \left(1 + \frac{\ell}{\mu}\right)^2\left(\frac{M\nu}{\mu} + \frac{M\rho^2}{\mu^2}\right) + \left(2 + \frac{5\ell}{\mu}\right)\left(1 + \frac{2\ell}{\mu}\right)\left(\frac{\ell\rho}{\mu} + \frac{M\rho^2}{\mu^2}\right) \\ & + \frac{2\ell\rho}{\mu^2}\left(1 + \frac{\ell}{\mu}\right)^2\left(\ell + \frac{M\rho}{\mu}\right) + \frac{14\ell\rho}{\mu^2}\left(1 + \frac{2\ell}{\mu}\right)\left(\frac{\ell}{\mu} + \frac{M\rho}{\mu^2}\right) + \frac{50\ell^2}{\mu^3}\left(\frac{M\nu}{\mu} + \rho\right) = \mathcal{O}(\kappa^5).\end{aligned}$$

[4] Indeed, by taking $\lambda > 1$, function $\mathcal{L}_\lambda^*(x)$ can be written as

$$\begin{aligned}\mathcal{L}_\lambda^*(x) &= \min_{y\in\mathbb{R}^{d_y}}\left(f(x,y) + \lambda\left(g(x,y) - \min_{z\in\mathbb{R}^{d_y}} g(x,z)\right)\right) = \min_{y\in\mathbb{R}^{d_y}}\left(\bar{f}(x,y) + \lambda\left(-\bar{f}(x,y) - \min_{z\in\mathbb{R}^{d_y}} -\bar{f}(x,z)\right)\right) \\ &= \min_{y\in\mathbb{R}^{d_y}}\left((1-\lambda)\bar{f}(x,y) + \lambda\max_{z\in\mathbb{R}^{d_y}}\bar{f}(x,z)\right) = (1-\lambda)\max_{y\in\mathbb{R}^{d_y}}\bar{f}(x,y) + \lambda\max_{z\in\mathbb{R}^{d_y}}\bar{f}(x,z) = \max_{y\in\mathbb{R}^{d_y}}\bar{f}(x,y),\end{aligned}$$

which reduces to the objective function $\bar{\Phi}(x)$ in minimax problem (8).

E.2 Proof of Theorem E.2

From Lemma E.1, setting $\lambda = \Theta\left(\max\{\kappa^2/\Delta,\ \kappa^3/\epsilon\}\right)$ leads to

- $\|\nabla\Phi(x) - \nabla\mathcal{L}_\lambda^*(x)\|_2 \le \mathcal{O}(\epsilon)$, for any $x \in \mathbb{R}^{d_x}$;
- $\mathcal{L}_\lambda^*(x_{\text{int}}) - \min_{x\in\mathbb{R}^{d_x}} \mathcal{L}_\lambda^*(x) \le \mathcal{O}(\Delta)$.

Thus, we only need to prove that RAF^{2}BA (in Algorithm 5) can find an ϵ-first order stationary point of $\mathcal{L}_\lambda^*(x)$ within the desired complexity.

Similar to Condition 3.1 (in Section B.1) for the analysis of RAHGD (in Algorithm 3) , we can show the following condition is guaranteed to hold after running AGD for sufficient iterations.

Condition E.5. *Let $w_{t,-1} = x_{t,-1}$ and denote $y^*(w_{t,k}) = \arg\min f(w_{t,k},\cdot) + \lambda g(w_{t,k},\cdot)$, $z^*(w_{t,k}) = \arg\min g(w_{t,k},\cdot)$. Then for some $\sigma > 0$ and $t = 0, 1, 2, \ldots$, we assume that the estimators $y_{t,k} \in \mathbb{R}^{d_y}$ and $z_{t,k} \in \mathbb{R}^{d_y}$ satisfy the conditions*

$$\|y_{t,k} - y^*(w_{t,k})\|_2 \le \frac{\sigma}{2(1+\lambda)\ell}, \quad \text{for each } k = -1, 0, 1, 2, \ldots \tag{46}$$

and

$$\|z_{t,k} - z^*(w_{t,k})\|_2 \le \frac{\sigma}{2\ell}, \quad \text{for each } k = -1, 0, 1, 2, \ldots \tag{47}$$

Under Condition E.5 and Assumption 2.3 we have the following lemma.

Lemma E.6. *Suppose Assumption 2.3 and Condition E.5 hold, then for each $k = -1, 0, 1, \ldots$, and $t = 0, 1, 2, \ldots$, we have*

$$\|u_{t,k} - \nabla\mathcal{L}_\lambda^*(w_{t,k})\|_2 \le \sigma \ ,$$

where $u_{t,k}$ is defined in line 9 in Algorithm 5.

Proof. Note that

$$u_{t,k} = \nabla_x f(w_{t,k}, y_{t,k}) + \lambda(\nabla_x g(w_{t,k}, y_{t,k}) - \nabla_x g(w_{t,k}, z_{t,k}))$$

and

$$\nabla\mathcal{L}_\lambda^*(w_{t,k}) = \nabla_x f(w_{t,k}, y^*(w_{t,k})) + \lambda(\nabla_x g(w_{t,k}, y^*(w_{t,k})) - \nabla_x g(w_{t,k}, z^*(w_{t,k})) \ .$$

Then from Condition E.5 and the Lipschitz continuity of gradient of f and g, we have

$$\|u_{t,k} - \nabla\mathcal{L}_\lambda^*(w_{t,k})\|_2 \le (1+\lambda)\ell \cdot \frac{\sigma}{2(1+\lambda)\ell} + \ell \cdot \frac{\sigma}{2\ell} = \sigma \ .$$

□

Note that the only difference of Algorithm 5 and Algorithm 3 is the construction for the inexact gradient of the objective functions, i.e., $\nabla\mathcal{L}_\lambda^*(w_{t,k}) \approx u_{t,k} = \nabla_x f(w_{t,k}, y_{t,k}) + \lambda(\nabla_x g(w_{t,k}, y_{t,k}) - \nabla_x g(w_{t,k}, z_{t,k}))$ for Algorithm 5 and $\nabla\Phi(w_{t,k}) \approx u_{t,k} = \nabla_x f(w_{t,k}, y_{t,k}) - \nabla^2_{xy} g(w_{t,k}, y_{t,k}) v_{t,k}$ for Algorithm 3. Thus, we can directly follow the proof of Theorem 3.4 by replacing $\Phi(x)$ by $\mathcal{L}_\lambda^*(x)$ and achive the following result.

Theorem E.7. *Suppose that Assumptions 2.3 and Condition E.5 hold. Denote $\Delta_\lambda = \mathcal{L}_\lambda^*(x_{\text{int}}) - \min_{x\in\mathbb{R}^{d_x}} \mathcal{L}_\lambda^*(x)$ and $\kappa' = (\lambda+1)\ell/(\lambda\mu - \ell)$ (recall our choice of $\lambda \ge 2\kappa$). Let*

$$\eta = \frac{1}{4L_\lambda}, \quad B = \sqrt{\frac{\epsilon}{\rho_\lambda}}, \quad \theta = 4(\rho_\lambda\epsilon\eta^2)^{1/4}, \quad K = \frac{1}{\theta}, \quad \alpha = \frac{1}{\ell}, \quad \beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1},$$
$$\alpha' = \frac{1}{(\lambda+1)\ell}, \quad \beta' = \frac{\sqrt{\kappa'}-1}{\sqrt{\kappa'}+1}, \quad \sigma = \epsilon^2$$

and assume that $\epsilon \le L_\lambda^2/\rho_\lambda$. Then our RAF^{2}BA in Algorithm 5 terminates within $\mathcal{O}(\Delta_\lambda L_\lambda^{0.5}\rho_\lambda^{0.25}\epsilon^{-1.75})$ iterates, outputting $\hat{w}$ satisfying $\|\nabla\mathcal{L}_\lambda^*(\hat{w})\|_2 \le 83\epsilon$.

Now we consider the overall inner loop iteration number from the step of AGD to achieve $z_{t,k}$ in the algorithm. Following the proof of Lemma B.6 (in Section B.2), we achieve the upper bound of $\|z^*(w_{t,-1})\|_2 \leq \hat{C}_z$ as follows.

Lemma E.8. *Consider the setting of Theorem E.7, and we run Algorithm 5, then we have*

$$\|z^*(w_{t,-1})\|_2 \leq \hat{C}_z$$

for any $t > 0$ and some constant $C > 0$, where $\hat{C}_z = \|z^*(x_{0,0})\|_2 + (2B + \eta\sigma + \eta C)\kappa\Delta_\lambda\sqrt{\rho_\lambda}\epsilon^{-3/2}$.

Taking

$$T_{t,k} = \begin{cases} \left\lceil 2\sqrt{\kappa}\log\left(\frac{2\ell\sqrt{\kappa+1}}{\sigma}\hat{C}_z\right)\right\rceil, & k = -1, \\ \left\lceil 2\sqrt{\kappa}\log\left(\frac{2\ell\sqrt{\kappa+1}}{\sigma}\left(\frac{\sigma}{2\ell} + 2\kappa B\right)\right)\right\rceil, & k \geq 0, \end{cases} \tag{48}$$

for Algorithm 5, we can use induction to show Lemma E.8 and equation (47) in Condition E.5 hold, which is similar to the analysis in Section B.2.

Finally, we consider the overall inner loop iteration number from the step of AGD to achieve $y_{t,k}$ in the algorithm. Following the proof of Lemma B.6 (in Section B.2), we achieve the upper bound of $\|y^*(w_{t,-1})\|_2 \leq \hat{C}_y$ as follows.

Lemma E.9. *Consider the setting of Theorem E.7, and we run Algorithm 5, then we have*

$$\|y^*(w_{t,-1})\|_2 \leq \hat{C}_y$$

for any $t = 0, 1, 2, \ldots$ and some constant $C > 0$, where $\hat{C}_y = \|y^*(x_{0,0})\|_2 + (2B + \eta\sigma + \eta C)\kappa'\Delta_\lambda\sqrt{\rho_\lambda}\epsilon^{-3/2}$.

Notice that the condition number of $f(x,\cdot) + \lambda g(x,\cdot)$ is $\kappa' = (\lambda+1)\ell/(\lambda\mu - \ell) = \mathcal{O}(\kappa)$ for any $x \in \mathbb{R}^{d_x}$. Analogizing the setting of $T_{t,k}$, we take

$$T'_{t,k} = \begin{cases} \left\lceil 2\sqrt{\kappa'}\log\left(\frac{2(1+\lambda)\ell\sqrt{\kappa'+1}}{\sigma}\hat{C}_y\right)\right\rceil, & k = -1, \\ \left\lceil 2\sqrt{\kappa'}\log\left(\frac{2(\lambda+1)\ell\sqrt{\kappa'+1}}{\sigma}\left(\frac{\sigma}{2(\lambda+1)\ell} + 2\kappa' B\right)\right)\right\rceil, & k \geq 0, \end{cases} \tag{49}$$

for Algorithm 5. We can also use induction to show Lemma E.9 and equation (46) in Condition E.5 hold, which is similar to the analysis in Section B.2.

Combining Theorem E.7 with the above settings of $T_{t,k}$ and $T'_{t,k}$, we can conclude that our `RAF`^{2}`BA` can find an ϵ-first-order stationary point of $\mathcal{L}^*_\lambda(x)$ (also an $\mathcal{O}(\epsilon)$-first-order stationary point of $\Phi(x)$) within oracle complexities $Gc(f,\epsilon) = Gc(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$, which is similar to the proof of Corollary 3.6 (in Section B.3).

E.3 Proof of Theorem E.3

From Lemma E.1, setting of $\lambda = \Theta\left(\max\{\kappa^2/\Delta,\ \kappa^3/\epsilon,\ \kappa^6/\sqrt{\epsilon}\}\right)$ leads to

- $\|\nabla\Phi(x) - \nabla\mathcal{L}^*_\lambda(x)\|_2 \leq \mathcal{O}(\epsilon)$, for any $x \in \mathbb{R}^{d_x}$;
- $\left\|\nabla^2\Phi(x) - \nabla^2\mathcal{L}^*_\lambda(x)\right\|_2 \leq \mathcal{O}(\sqrt{\epsilon}\,)$, for any $x \in \mathbb{R}^{d_x}$;
- $\mathcal{L}^*_\lambda(x_{\text{int}}) - \min_{x\in\mathbb{R}^{d_x}}\ \mathcal{L}^*_\lambda(x) \leq \mathcal{O}(\Delta)$.

Now all we need is to show that our `PRAF`^{2}`BA` can find an $(\epsilon, O(\kappa^{2.5}\sqrt{\epsilon}\,))$-second-order stationary point of $\mathcal{L}^*_\lambda(x)$ within the desired complexity.

Following the proof of Theorem 4.1, we have the following theorem.

Theorem E.10. *Suppose that Assumption 2.3 and Condition E.5 hold. We denote $\Delta_\lambda = \mathcal{L}^*_\lambda(x_{\text{int}}) - \min_{x\in\mathbb{R}^{d_x}}\mathcal{L}^*_\lambda(x)$ and $\kappa' = (\lambda+1)\ell/(\lambda\mu-\ell)$ and let*

$$\chi = \mathcal{O}\left(\log\frac{d_x}{\zeta\epsilon}\right), \quad \eta = \frac{1}{4L_\lambda}, \quad K = \frac{2\chi}{\theta}, \quad B = \frac{1}{288\chi^2}\sqrt{\frac{\epsilon}{\rho_\lambda}}, \quad \theta = \frac{1}{2}(\rho_\lambda\epsilon\eta^2)^{1/4}, \quad \sigma = \min\left\{\frac{\rho_\lambda B\zeta r\theta}{2\sqrt{d_x}}, \epsilon^2\right\},$$

$$\alpha = \frac{1}{\ell}, \quad \beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}, \quad \alpha' = \frac{1}{(\lambda+1)\ell}, \quad \beta' = \frac{\sqrt{\kappa'}-1}{\sqrt{\kappa'}+1}, \quad r = \min\left\{\frac{L_\lambda B^2}{4C}, \frac{B+B^2}{\sqrt{2}}, \frac{\theta B}{20K}, \sqrt{\frac{\theta B^2}{2K}}\right\},$$

for some positive constant C, where we assume that $\epsilon \leq L_\lambda^2/\rho_\lambda$. Then `PRAF`^{2}`BA` *in Algorithm 5 terminates in at most $\mathcal{O}\big(\Delta_\lambda L_\lambda^{0.5}\rho_\lambda^{0.25}\chi^6 \cdot \epsilon^{-1.75}\big)$ iterations and the output satisfies $\|\nabla \mathcal{L}_\lambda^*(\hat{w})\|_2 \leq \epsilon$ and $\lambda_{\min}(\nabla^2 \mathcal{L}_\lambda^*(\hat{w})) \geq -1.011\sqrt{\rho_\lambda \epsilon}$ with probability at least $1-\zeta$.*

Now we set parameters $T_{t,k}$ and $T'_{t,k}$ by the similar way to the counterparts in Section C.2 and E.2, that is

$$T_{t,k} = \begin{cases} \left\lceil 2\sqrt{\kappa}\log\left(\frac{2\ell\sqrt{\kappa}+1}{\sigma}\tilde{C}_z\right)\right\rceil, & k=-1, \\ \left\lceil 2\sqrt{\kappa}\log\left(\frac{2\ell\sqrt{\kappa}+1}{\sigma}\left(\frac{\sigma}{2\ell}+2\kappa B\right)\right)\right\rceil, & k \geq 0, \end{cases} \tag{50}$$

and

$$T'_{t,k} = \begin{cases} \left\lceil 2\sqrt{\kappa'}\log\left(\frac{2(1+\lambda)\ell\sqrt{\kappa'}+1}{\sigma}\tilde{C}_y\right)\right\rceil, & k=-1, \\ \left\lceil 2\sqrt{\kappa'}\log\left(\frac{2(\lambda+1)\ell\sqrt{\kappa'}+1}{\sigma}\left(\frac{\sigma}{2(\lambda+1)\ell}+2\kappa' B\right)\right)\right\rceil, & k \geq 0, \end{cases} \tag{51}$$

where

$$\tilde{C}_z = \|z^*(x_{0,0})\|_2 + (2B+B^2+\eta\sigma+\eta C)\kappa\Delta_\lambda\sqrt{\rho_\lambda}\epsilon^{-3/2}$$

and

$$\tilde{C}_y = \|y^*(x_{0,0})\|_2 + (2B+B^2+\eta\sigma+\eta C)\kappa'\Delta_\lambda\sqrt{\rho_\lambda}\epsilon^{-3/2}.$$

We can also use induction to prove that Condition E.5 will hold when we choose $T_{t,k}$ and $T'_{t,k}$ as set in equation (50) and equation (51).

Combining Theorem E.10 with the above settings of $T_{t,k}$ and $T'_{t,k}$, we can conclude that our `PRAF`^{2}`BA` can find an $(\epsilon, \kappa^{2.5}\mathcal{O}(\sqrt{\epsilon}))$-second-order stationary point of $\mathcal{L}_\lambda^*(x)$ (also an $(\mathcal{O}(\epsilon), \kappa^{2.5}\mathcal{O}(\sqrt{\epsilon}))$-second-order stationary point of $\Phi(x)$) within oracle complexities $Gc(f,\epsilon) = Gc(g,\epsilon) = \tilde{\mathcal{O}}(\kappa^{3.25}\epsilon^{-1.75})$, which is similar to the proof of Corollary 4.3 (in Section C.3).

F Empirical Studies

We conducted a series of experiments to validate the theoretical contributions presented in this paper. Specifically, we evaluated the effectiveness of our proposed algorithms, `RAHGD`, `PRAHGD`, `RAF`^{2}`BA` and `PRAF`^{2}`BA`, by applying them to two different tasks: data hyper-cleaning for the MNIST dataset and hyperparameter optimization of logistic regression for the 20 News Group dataset. Our experiments demonstrate that our algorithms outperform several established baseline algorithms, such as BA, AID-BiO, ITD-BiO, and PAID-BiO, with much faster convergence rates. Additionally, we conducted a synthetic minimax problem experiment, showing that our `PRAGDA` algorithm exhibits a faster convergence rate when compared to iMCN.

F.1 Synthetic Minimax Problem

We construct the following nonconvex-strong-concave minimax problem:

$$\min_{x\in\mathbb{R}^3}\max_{y\in\mathbb{R}^2} f(x,y) = w(x_3) - 10y_1^2 + x_1y_1 - 5y_2^2 + x_2y_2,$$

where $x = [x_1, x_2, x_3]^T$ and $y = [y_1, y_2]^T$ and

$$w(x) = \begin{cases} \sqrt{\epsilon}(x+(L+1)\sqrt{\epsilon})^2 - \frac{1}{3}(x+(L+1)\sqrt{\epsilon})^3 - \frac{1}{3}(3L+1)\epsilon^{3/2}, & x \leq -L\sqrt{\epsilon}; \\ \epsilon x + \frac{\epsilon^{3/2}}{3}, & -L\sqrt{\epsilon} < x \leq -\sqrt{\epsilon}; \\ -\sqrt{\epsilon}x^2 - \frac{x^3}{3}, & -\sqrt{\epsilon} < x \leq 0; \\ -\sqrt{\epsilon}x^2 + \frac{x^3}{3}, & 0 < x \leq \sqrt{\epsilon}; \\ -\epsilon x + \frac{\epsilon^{3/2}}{3}, & \sqrt{\epsilon} < x \leq L\sqrt{\epsilon}; \\ \sqrt{\epsilon}(x-(L+1)\sqrt{\epsilon})^2 + \frac{1}{3}(x-(L+1)\sqrt{\epsilon})^3 - \frac{1}{3}(3L+1)\epsilon^{3/2}, & L\sqrt{\epsilon} < x; \end{cases}$$

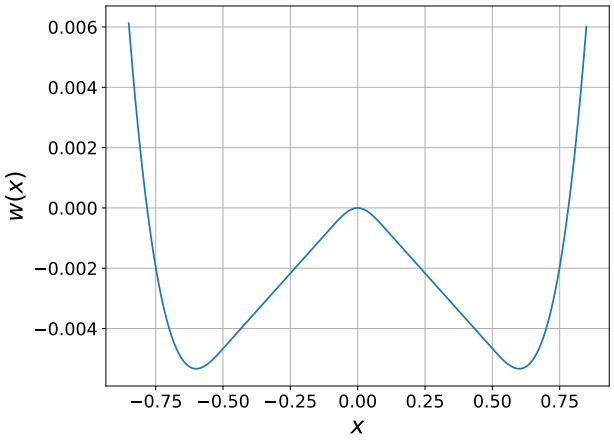
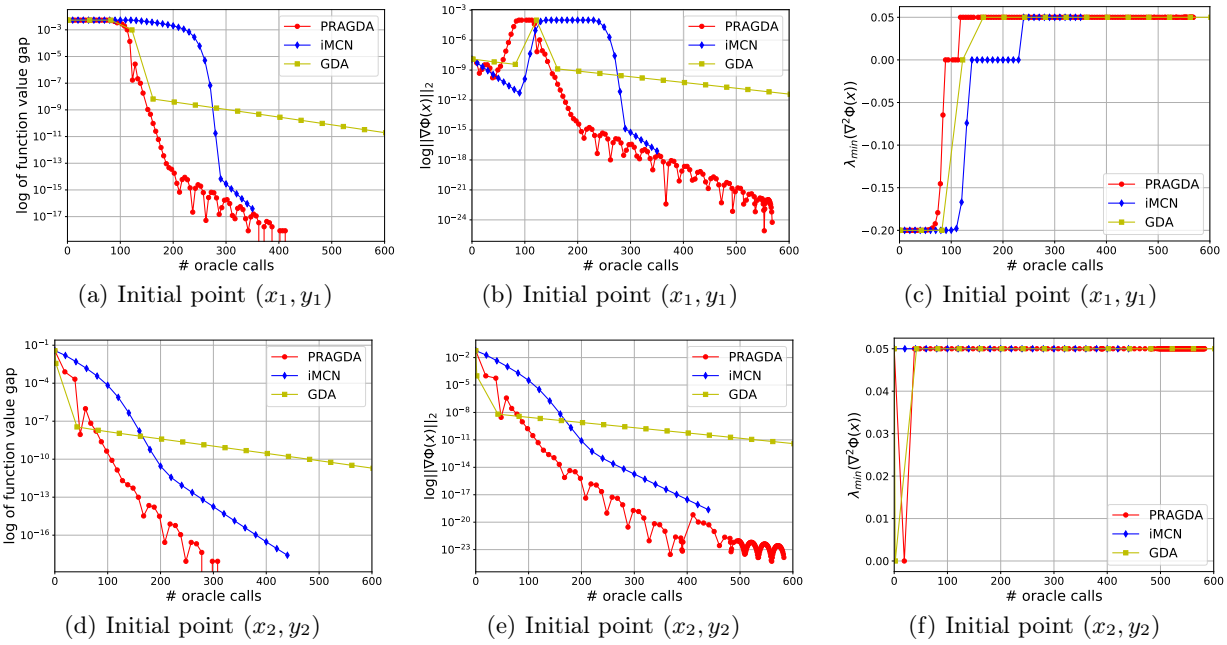


Figure 2: W-shape function (Tripuraneni et al., 2018)



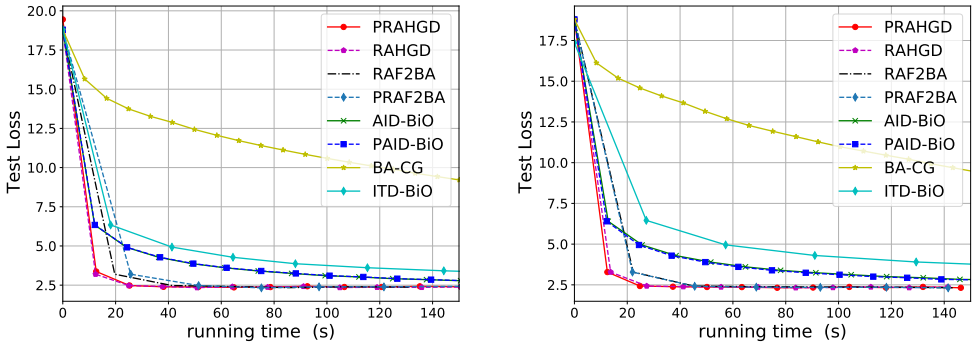
(a) Initial point (x_1, y_1) (b) Initial point (x_1, y_1) (c) Initial point (x_1, y_1)

(d) Initial point (x_2, y_2) (e) Initial point (x_2, y_2) (f) Initial point (x_2, y_2)

Figure 3: A selection of empirical results with convergence measured by both the function value gap, gradient norm and minimal eigenvalue of Hessian (in absolute value), applied on the task of the synthetic minimax problem.

is the W-shape-function (Tripuraneni et al., 2018) and we set $\epsilon = 0.01, L = 5$ in our experiment. We visualize the $w(\cdot)$ in Figure 2. It is straightforward to verify that $[x_0; y_0] = [[0, 0, 0]^\top; [0, 0]^\top]$ is a saddle point of $f(x, y)$. We construct our experiment with two different initial points: $[x_1; y_1] = \left[[10^{-3}, 10^{-3}, 10^{-16}]^\top; [0, 0]^\top\right]$ and $[x_2, y_2] = \left[[0, 0, 1]^\top; [0, 0]^\top\right]$. Note that $[x_1; y_1]$ is relatively close to initialization $[x_0; y_0]$, while $[x_2; y_2]$ is relatively distant from $[x_0; y_0]$. We numerically compare our `PRAGDA` with the iMCN (Luo et al., 2022) algorithm and classical GDA (Lin et al., 2020b) algorithm. The results are shown in Figure 3 where a grid search is adopted to choose the learning rate of AGD steps, GDA, and outer-loop learning rate of `PRAGDA`. The grids are for learning rates $\{c \times 10^i : c \in \{1, 5\}, i \in \{1, 2, 3\}\}$ and momentum parameters $\{c \times 0.1 : c \in \{1, 2, 3, 4, 5, 6, 7, 8, 9\}\}$.

We compare the number of oracle calls against $\Phi(x) - \Phi(x^*)$, $\|\nabla\Phi(x)\|$ and $\lambda_{\min}(\nabla^2\Phi(x))$ and plot the results in Figure 3. From the curves corresponding to initial point (x_2, y_2), we observe that all the three algorithms converge to the minimum when the initial point is far from the strict saddle point, but our `PRAGDA` converges much faster than iMCN and GDA. When the initial point is close to the strict saddle point, Figure 3(b) shows that the GDA algorithm gets stuck at the strict saddle point since its Hessian minimum eigenvalue are always



(a) Corruption rate $p = 0.2$ (b) Corruption rate $p = 0.4$

Figure 4: Comparison of various bilevel algorithms for data hypercleaning at different corruption rates

negative. However, our `PRAGDA` and iMCN can reach the points which have positive Hessian minimum eigenvalues. Also, our `PRAGDA` converges faster than iMCN.

F.2 Data Hypercleaning

Data hypercleaning (Franceschi et al., 2017; Shaban et al., 2019) is an application example of bilevel optimization. In practice, we may have a dataset with label noise and we require some time or cost to clean up a subset of the noisy data. To train a model in such a setting, we can treat the cleaned data as the validation set and the rest data as the training set. Then it can be transferred into a bilevel optimization:

$$\begin{aligned} &\min_{\lambda \in \mathbb{R}^{|\mathcal{D}_{\text{tr}}|}} f(W^*(\lambda), \lambda) \triangleq \frac{1}{|\mathcal{D}_{\text{val}}|} \sum_{(x_i, y_i) \in \mathcal{D}_{\text{val}}} -\log(y_i^\top W^*(\lambda) x_i) \\ &\text{s.t.} \quad W^*(\lambda) = \underset{W \in \mathbb{R}^{d_y \times d_x}}{\arg\min} \; g(W, \lambda) \triangleq \frac{1}{|\mathcal{D}_{\text{tr}}|} \sum_{(x_i, y_i) \in \mathcal{D}_{\text{tr}}} -\sigma(\lambda_i) \log(y_i^\top W x_i) + C_r ||W||^2 \;, \end{aligned} \tag{52}$$

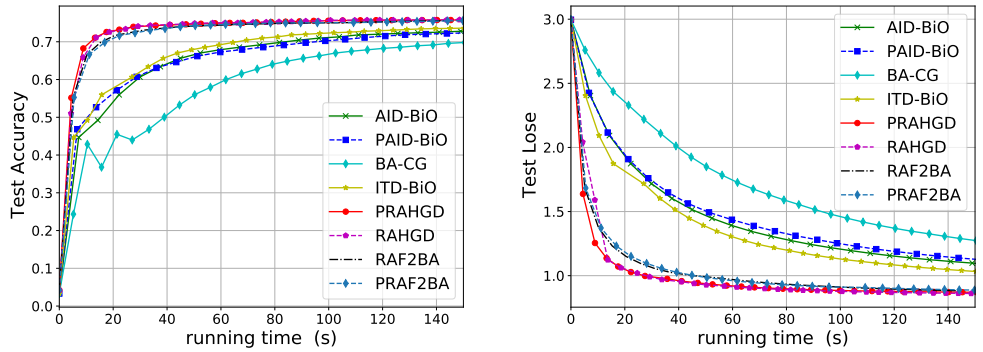
where $\mathcal{D}_{\text{tr}} = \{(x_i, y_i)\}$ is the training dataset, $\mathcal{D}_{\text{val}} = \{(x_i, y_i)\}$ is the validation dataset, W is the weight of the classifier, $\lambda_i \in \mathbb{R}$, $\sigma(\cdot)$ is the sigmoid function and C_r is a regularization parameter. Following Shaban et al. (2019) and Ji et al. (2021), we choose $C_r = 0.001$.

We conducted an experiment on MNIST (LeCun et al., 1998), which has $d_x = 785$ and $d_y = 10$ for problem (52). The training set contains $|\mathcal{D}_{\text{tr}}| = 20,000$ images, some of which have their labels randomly disrupted. We refer to the ratio of images with disrupted labels as the corruption rate p. The validation set contains $|\mathcal{D}_{\text{val}}| = 5,000$ images with correct labels, and the testing set consists of 10,000 images.

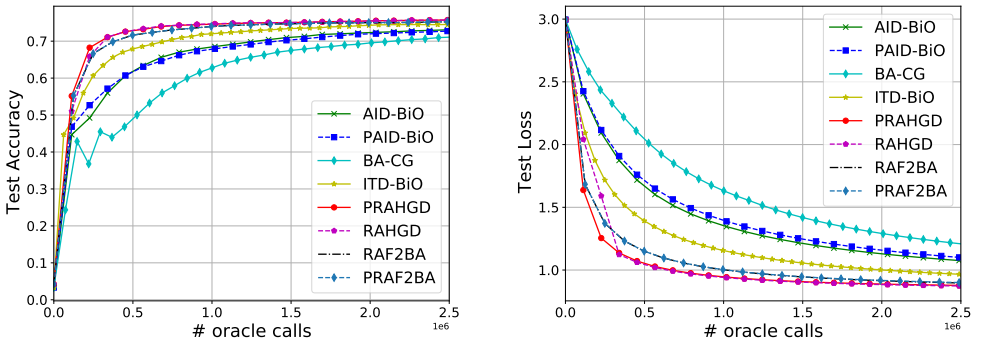
The experimental results are shown in Figure 4. For the BA algorithm proposed by Ghadimi & Wang (2018), we also use the conjugate gradient descent method to compute the Hessian vector since they did *not* specify it and we called it BA-CG in Figure 4. For all algorithms, We choose the inner-loop learning rate and outer-loop learning rate from $\{0.001, 0.01, 0.1, 1, 10\}$ and the iteration number of CG step from $\{3, 6, 12, 24\}$. For all algorithms except BA, we choose the iteration number of GD or AGD steps from $\{50, 100, 200, 500, 1000\}$ and for BA algorithm, as adopted by Ghadimi & Wang (2018), we choose the iteration number of GD steps from $\{\lceil c(k+1)^{1/4} \rceil : c \in \{0.5, 1, 2, 4\}\}$. For `RAF`^{2}`BA` and `PRAF`^{2}`BA`, we choose λ (in equation (42)) from $\{100, 300, 500, 700\}$. We observe that our `RAHGD`, `PRAHGD`, `RAF`^{2}`BA` and `PRAF`^{2}`BA` converge faster than rival algorithms.

F.3 Hyperparameter Optimization

Hyperparameter optimization is a classical machine learning problem that can be formulated as bilevel optimization. The goal of hyperparameter optimization is to find the optimal hyperparameter to minimize the loss on the validation dataset. We compare the performance of our algorithm `RAHGD` and `PRAHGD` with the baseline algorithms listed in Table 1 and Table 2 over a logistic regression problem on 20 News group dataset (Grazzi et al., 2020). This dataset consists of 18,846 news items divided into 20 topics, and features include 130,170 tf-idf sparse vectors.



(a) testing accuracy vs. running time (b) testing lose vs. running time



(c) testing accuracy vs. number of oracle calls (d) testing lose vs. number of oracle calls

Figure 5: Comparison of various bilevel algorithms on logistic regression on 20 Newsgroup dataset. Figures (a) and (b) show the results of testing accuracy and testing lose vs. running time respectively. Figures (c) and (d) show the results of testing accuracy and testing loss vs. number of oracles calls respectively.

We divided the data into three parts: $|\mathcal{D}_{\text{tr}}| = 5,657$ samples for training, $|\mathcal{D}_{\text{val}}| = 5,657$ samples for validation, and 7,532 samples for testing. Then the objective function of this problem can be written in the following form.

$$\min_{\lambda \in \mathbb{R}^p} \frac{1}{|\mathcal{D}_{\text{val}}|} \sum_{(x_i,y_i)\in\mathcal{D}_{\text{val}}} L(w^*(\lambda); x_i, y_i),$$

$$\text{s.t.} \quad w^*(\lambda) = \arg\min_{w \in \mathbb{R}^{c\times p}} \frac{1}{|\mathcal{D}_{\text{tr}}|} \sum_{(x_i,y_i)\in\mathcal{D}_{\text{tr}}} L(w; x_i, y_i) + \frac{1}{2cp} \sum_{j=1}^{c} \sum_{k=1}^{p} \exp(\lambda_k) w_{jk}^2,$$

where $\mathcal{D}_{\text{tr}} = \{(x_i, y_i)\}$ is the training dataset, $\mathcal{D}_{\text{val}} = \{(x_i, y_i)\}$ is the validation dataset, L is the cross-entropy loss function, $c = 20$ is the number of topics and $p = 130,170$ is the dimension of features. Analogous to Section F.2, we use the conjugate gradient descent method to approximate the Hessian vector.

For all algorithms listed in Figure 5, we choose the inner-loop learning rate and outer-loop learning rate from $\{0.001, 0.01, 0.1, 1, 10, 100, 1000\}$, where the iteration number of GD or AGD step is chosen from $\{5, 10, 30, 50\}$ and the iteration number of CG step from $\{5, 10, 30, 50\}$. For BA-CG, we choose the iteration number of GD steps from $\{\lceil c(k+1)^{1/4} \rceil : c \in \{0.5, 1, 2, 4\}\}$, as is adopted by Ghadimi & Wang (2018). For `RAF`^{2}`BA`, we choose λ (in equation (42)) from $\{100, 300, 500, 700\}$. The results are shown in Figure 5. We observe that our `RAHGD`, `PRAHGD`, `RAF`^{2}`BA` and `PRAF`^{2}`BA` converge faster than rival algorithms.