A Constrained Optimization Approach to Bilevel Optimization with Multiple Inner Minima

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Abstract

Bilevel optimization has found extensive applications in modern machine learning problems such as hyperparameter optimization, neural architecture search, meta-learning, etc. While bilevel problems with a unique inner minimal point (e.g., where the inner function is strongly convex) are well understood, bilevel problems with multiple inner minimal points remains to be a challenging and open problem. Existing algorithms designed for such a problem were applicable to restricted situations and do not come with the full guarantee of convergence. In this paper, we propose a new approach, which convert the bilevel problem to an equivalent constrained optimization, and then the primal-dual algorithm can be used to solve the problem. Such an approach enjoys a few advantages including (a) addresses the multiple inner minima challenge; (b) features fully first-order efficiency without involving second-order Hessian and Jacobian computations, as opposed to most existing gradient-based bilevel algorithms; (c) admits the convergence guarantee via constrained nonconvex optimization. Our experiments further demonstrate the desired performance of the proposed approach.

1 Introduction

Bilevel optimization has received intensive attention recently due to its applications in a variety of modern machine learning problems. Typically, parameters handled by bilevel optimization are divided into two different types such as meta and base learners in few-shot meta-learning \cite{Bertinetto et al. 2018, Rajeswaran et al. 2019}, hyperparameters and model parameters training in automated hyperparameter tuning \cite{Franceschi et al. 2018, Shaban et al. 2019}, actors and critics in reinforcement learning \cite{Konda & Tsitsiklis 2000, Hong et al. 2020}, and model architectures and weights in neural architecture search \cite{Liu et al. 2018}.

Mathematically, bilevel optimization captures intrinsic hierarchical structures in those machine learning models, and can be formulated into the following two-level problem:

\begin{equation}
\min_{x \in X, y \in S_x} f(x, y) \quad \text{with} \quad S_x = \arg \min_{y \in Y} g(x, y),
\end{equation}

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where \( f(x, y) \) and \( g(x, y) \), the outer- and inner-level objective functions, are continuously differentiable, and the supports \( \mathcal{X} \subseteq \mathbb{R}^p \) and \( \mathcal{Y} \subseteq \mathbb{R}^d \) are convex and closed. For a fixed \( x \in \mathcal{X} \), \( S_x \) is the set of all \( y \in \mathcal{Y} \) that yields the minimal value of \( g(x, \cdot) \).

A broad collection of approaches have been proposed to solve the bilevel problem in eq. (1). Among them, gradient based algorithms have shown great effectiveness and efficiency in various deep learning applications, which include approximated implicit differentiation (AID) based methods (Domke, 2012; Pedregosa, 2016; Gould et al., 2016; Liao et al., 2018; Lorraine et al., 2020; Ji et al., 2021) and iterative differentiation (ITD) (or dynamic system) based methods (Maclaurin et al., 2015; Franceschi et al., 2017; Shaban et al., 2019; Grazzi et al., 2020b; Liu et al., 2020; 2021a). Many stochastic bilevel algorithms have been proposed recently via stochastic gradients (Ghadimi & Wang, 2018; Hong et al., 2020; Ji et al., 2021), and variance reduction (Yang et al., 2021) and momentum (Chen et al., 2021; Khanduri et al., 2021; Guo & Yang, 2021).

Most of these studies rely on the simplification that for each outer variable \( x \), the inner-level problem has a \textbf{single} global minimal point. The studies for a more challenging scenario with \textbf{multiple} inner-level solutions (i.e., \( S_x \) has multiple elements) are rather limited. In fact, a counter example has been provided in (Liu et al., 2020) to illustrate that simply applying algorithms designed for the single inner minima case will fail to optimize bilevel problems with multiple inner minima. Thus, bilevel problems with multiple inner minima deserve serious efforts of exploration. Recently, Liu et al. (2020; Li et al., 2020; Liu et al., 2021a) proposed a gradient aggregation method and Liu et al. (2021a) proposed a value-function-based method from a constrained optimization view to address the issue of multiple inner minima. However, all of these approaches take a \textit{double-level} optimization structure, updating the outer variable \( x \) after fully updating \( y \) over the inner and outer functions, which could lose efficiency and cause difficulty in implementations. Further, these approaches have been provided with only the \textit{asymptotic} convergence guarantee without characterization of the convergence rate.

The focus of this paper is to develop a better-structured bilevel optimization algorithm, which handles the multiple inner minima challenge and comes with a finite-time convergence rate guarantee.

### 1.1 Our Contributions

In this paper, we propose a novel constrained optimization approach for bilevel optimization. Our design features 1) an equivalent single-level (treating \( x \) and \( y \) as a single updating variable) constrained optimization reformulation of bilevel problems to avoid the direct characterization of the solution set \( S_x \), and 2) a novel primal-dual bilevel algorithm which provably converges to an \( \epsilon \)-accurate KKT point. The specific contributions are summarized as follows.

**Algorithmic design.** We first propose a simple and easy-to-implement primal-dual bilevel optimizer (PDBO), which has guaranteed convergence w.r.t. the dual problem. We further propose a proximal version of PDBO (Proximal-PDBO), which achieves a stronger convergence guarantee to the KKT point as we further discuss below. Differently from existing bilevel methods designed for handling multiple inner minima in Liu et al. (2020; Li et al. (2020; Liu et al. (2021a) that update variables \( x \) and \( y \) in a \textit{nested} manner, both PDBO and Proximal-PDBO update \( x \) and \( y \) simultaneously as a single variable \( z \) and hence admit a much simpler implementation. In addition, both algorithms do not involve any second-order information of the inner and outer functions \( f \) and \( g \), as opposed to many AID- and ITD-based approaches, and hence are computationally more efficient.

**Convergence rate analysis.** We provide the first-known convergence rate analysis for bilevel optimization with multiple inner-level minima. We show that the proposed Proximal-PDBO achieves an \( \epsilon \)-KKT point of the equivalent constrained optimization problem for any arbitrary \( \epsilon > 0 \) with a sublinear convergence rate.
Here, the KKT condition serves as a necessary condition for the global optimality of constrained optimization (and hence the corresponding bilevel problem). Technically, the constrained nonconvex optimization problem here is more challenging than the standard formulation studied in Boob et al. (2019); Ma et al. (2020) due to the nature of bilevel optimization. Specifically, our analysis needs to deal with the bias errors arising in gradient estimations for the updates of both the primal and dual variables. Further, we establish a uniform upper bound on optimal dual variables, which was taken as an assumption in the standard analysis in Boob et al. (2019).

**Empirical performance.** In the synthetic experiment with intrinsic multiple inner solutions, we show that our algorithm converges to the global minimizer, whereas AID- and ITD-based methods are stuck in local minima. We further demonstrate the effectiveness and better performance of our algorithm in hyperparameter optimization.

### 1.2 Related Works

**Bilevel optimization via AID and ITD.** AID and ITD are two popular approaches to reduce the computational challenging in approximating the outer-level gradient (which is often called hypergradient in the literature). In particular, AID-based bilevel algorithms (Domke, 2012; Pedregosa, 2016; Gould et al., 2016; Liao et al., 2018; Grazzi et al., 2020b; Lorraine et al., 2020; Ji & Liang, 2021; MacKay et al., 2019) approximate the hypergradient efficiently via implicit differentiation combined with a linear system solver. ITD-based approaches (Domke, 2012; Maclaurin et al., 2015; Franceschi et al., 2017, 2018; Shaban et al., 2019; Grazzi et al., 2020b; MacKay et al., 2019) approximate the inner-level problem using a dynamic system. For example, Franceschi et al. (2017, 2018) computed the hypergradient via reverse or forward mode in automatic differentiation. This paper proposes a novel constrained optimization based approach for bilevel optimization.

**Optimization theory for bilevel optimization.** Some works such as (Franceschi et al., 2018; Shaban et al., 2019) analyzed the asymptotic convergence performance of AID- and ITD-based bilevel algorithms. Ghadimi & Wang (2018) provided convergence rate analysis for various AID- and ITD-based approaches and their variants in applications such as meta-learning. (Hong et al., 2020; Ji et al., 2021; Yang et al., 2021; Khanduri et al., 2021) developed convergence rate analysis for their proposed stochastic bilevel optimizers. This paper provides the first-known convergence rate analysis for the setting with multiple inner minima.

**Bilevel optimization with multiple inner minima.** Sabach & Shtern (2017) proposed a bilevel gradient sequential averaging method (BiG-SAM) for single-variable bilevel optimization (i.e., without variable $x$), and provided an asymptotic convergence analysis for this algorithm. Liu et al. (2020) Li et al. (2020) uses an idea similar to BiG-SAM, and proposed a gradient aggregation approach for the general bilevel problem in eq. (1) with an asymptotic convergence guarantee. Liu et al. (2021b) proposed an initialization auxiliary algorithm for the bilevel problems with a nonconvex inner objective function.

Highly relevant to our study is the work by Liu et al. (2021a) which also proposed a constrained optimization method for bilevel optimization. As a comparison, our method has three major differences. First, the problem formulation in Liu et al. (2021a) takes a double-level structure, which updates the outer variable $x$ after fully updating $y$ over the inner and outer functions, whereas our formulation takes a single-level structure, treating both $x$ and $y$ together as a single updating variable $z$ in constrained optimization. Second, Liu et al. (2021a) uses the log-barrier interior-point method for solving constrained optimization, whereas we adopt a primal-dual algorithmic design. Third, Liu et al. (2021a) provided an asymptotic convergence guarantee for...
their algorithm, whereas we characterize the finite-time convergence rate for our algorithm.

## 2 Problem Formulation

We study a bilevel optimization problem given in eq. (1), which is restated below

\[
\min_{x \in \mathcal{X}, y \in \mathcal{S}_x} f(x, y) \quad \text{with} \quad \mathcal{S}_x = \arg \min_{y \in \mathcal{Y}} g(x, y),
\]

where the outer- and inner-level objective functions \( f(x, y) \) and \( g(x, y) \) are continuously differentiable, and the supports \( \mathcal{X} \) and \( \mathcal{Y} \) are convex and closed subsets of \( \mathbb{R}^p \) and \( \mathbb{R}^d \), respectively. For a fixed \( x \in \mathcal{X} \), \( \mathcal{S}_x \) is the set of all \( y \in \mathcal{Y} \) that yields the minimal value of \( g(x, \cdot) \). In this paper, we consider the following assumed function geometries.

**Assumption 1.** The inner function \( g(x, y) \) is convex with respect to \( y \) for any fixed \( x \in \mathcal{X} \).

The convexity assumption on \( g(x, y) \) still allows the inner function \( g(x, \cdot) \) to have multiple global minimal points, and the challenge for bilevel algorithm design due to multiple inner minima still remains. Further, the set \( \mathcal{S}_x \) of minimizers is convex due to convexity of \( g(x, y) \) w.r.t. \( y \). We note that \( g(x, \cdot) \) w.r.t. \( x \) and the outer function \( f(x, y) \) can be nonconvex in general.

We further take the following standard assumptions on the inner and outer objective functions.

**Assumption 2 (Smoothness conditions).** The objective functions \( f(x, y) \) and \( g(x, y) \) are

- **Lipschitz continuous:** for any \( x, \tilde{x} \in \mathcal{X} \) and \( y, \tilde{y} \in \mathcal{Y} \),
  \[
  |f(x, y) - f(\tilde{x}, \tilde{y})| \leq L_f \sqrt{\|x - \tilde{x}\|^2 + \|y - \tilde{y}\|^2},
  \]
  \[
  |g(x, y) - g(\tilde{x}, \tilde{y})| \leq L_g \sqrt{\|x - \tilde{x}\|^2 + \|y - \tilde{y}\|^2}.
  \]

- **Gradient Lipschitz:** for any \( x, \tilde{x} \in \mathcal{X} \) and \( y, \tilde{y} \in \mathcal{Y} \),
  \[
  \|\nabla f(x, y) - \nabla f(\tilde{x}, \tilde{y})\|_2 \leq \rho_f \sqrt{\|x - \tilde{x}\|^2 + \|y - \tilde{y}\|^2},
  \]
  \[
  \|\nabla g(x, y) - \nabla g(\tilde{x}, \tilde{y})\|_2 \leq \rho_g \sqrt{\|x - \tilde{x}\|^2 + \|y - \tilde{y}\|^2}.
  \]

## 3 Proposed Approach and Algorithm

In this section, we formally describe our approach for solving the bilevel problem in eq. (1). Our key idea is to transform the problem in eq. (1) into an equivalent single-level constrained optimization problem, and then leverage the primal-dual method for developing efficient algorithms.

### 3.1 A Constrained Optimization Approach

To solve the bilevel problem in eq. (1), one challenge is that it is not easy to explicitly characterize the set \( \mathcal{S}_x \) of the minimal points of \( g(x, y) \). This motivates the idea to describe such a set implicitly via a constraint. Clearly, the set \( \mathcal{S}_x \) can be described as \( \mathcal{S}_x = \{y \in \mathcal{Y} : g(x, y) \leq g^*(x)\} \), where \( g^*(x) := \min_{y \in \mathcal{Y}} g(x, y) \). In
this way, we can convert the bilevel problem in eq. (1) equivalently to the following constrained optimization problem:

$$\min_{x \in \mathcal{X}, y \in \mathcal{Y}} f(x, y) \quad \text{s.t.} \quad g(x, y) \leq g^*(x).$$

Since $g(x, y)$ is convex with respect to $y$, $g^*(x)$ in the constraint can be obtained efficiently via various convex minimization algorithms such as gradient descent.

To further simplify the notation, we let $z = (x, y) \in \mathbb{R}^{p+d}$, $Z = \mathcal{X} \times \mathcal{Y}$, $f(z) := f(x, y)$, $g(z) := g(x, y)$, and $g^*(z) := g^*(x)$, and then express the problem as follows.

$$\min_{z \in Z} f(z) \quad \text{s.t.} \quad h(z) := g(z) - g^*(z) \leq 0. \quad (2)$$

Thus, solving the bilevel problem in eq. (1) is converted to solving an equivalent single-level optimization in eq. (2).

Comparing to the constrained optimization approach proposed by Liu et al. 2021a, our method has three major differences. First, the problem formulation in Liu et al. 2021a takes a double-level structure, where the inner level is a constrained optimization problem w.r.t. inner variable $y$ for a given $x$ and the outer level is then to optimize over $x$. However, our formulation in eq. (2) takes a single-level structure, treating both $x$ and $y$ together as a single updating variable $z$ in constrained optimization. Second, Liu et al. 2021a uses the log-barrier interior-point method to solve constrained optimization, whereas we will adopt a primal-dual algorithmic design as we will present in Sections 3.2 and 3.3. Third, Liu et al. 2021a provided an asymptotic convergence guarantee for their algorithm, whereas we will characterize the convergence rate for our algorithm in Section 4.

To enable the algorithm design for the constrained optimization problem in eq. (2), we first make two standard changes to the constraint function. (i) Smoothing constraint: The constraint is nonsmooth, i.e., $g^*(z) := g^*(x)$ is nonsmooth in general, so that the design of gradient algorithm is not direct. We thus relax the constraint by replacing $g^*(z)$ with a smooth term

$$\tilde{g}^*(z) := \tilde{g}^*(x) = \min_{y \in \mathcal{Y}} \{ \tilde{g}(x, y) := g(x, y) + \frac{\alpha}{2} \|y\|^2 \},$$

where $\alpha > 0$ is a prescribed constant. It can be shown that for a given $x$, $\tilde{g}(x, y)$ has a unique minimal point, and the function $\tilde{g}^*(x)$ becomes differentiable with respect to $x$. Thus, the constraint becomes $g(z) - \tilde{g}^*(z) \leq 0$, which is differentiable. (ii) Strict feasibility: The constraint is not a strictly feasible function, i.e., the constraint cannot be satisfied with strict inequality (only with equality), in which case the convergence guarantee of the primal-dual algorithm can be difficult. We hence further relax the constraint by introducing a positive constant $\delta$ so that the constraint becomes $g(z) - \tilde{g}^*(z) - \delta \leq 0$ that admits strict feasible points.

Thus, our algorithm design in the next two subsections will be based on the following constrained optimization problem

$$\min_{z \in Z} f(z) \quad \text{s.t.} \quad \tilde{h}(z) := g(z) - \tilde{g}^*(z) - \delta \leq 0. \quad (3)$$

### 3.2 Primal-Dual Bilevel Optimizer (PDBO)

To solve the constrained optimization problem in eq. (3), we employ the primal-dual approach. The idea is to consider the following dual problem

$$\max_{\lambda \geq 0} \min_{z \in Z} \mathcal{L}(z, \lambda) = f(z) + \lambda \tilde{h}(z), \quad (4)$$

5
Algorithm 1 Primal-Dual Bilevel Optimizer (PDBO)

1: **Input:** stepsizes $\gamma$, $\beta$, initialization $z_0, \lambda_0$, and number $T$ of iterations
2: for $t = 0, 1, \ldots, T - 1$ do
3: Conduct projected gradient descent in eq. (6) for $N$ times with any given $\hat{y}_t$ as initialization
4: Update $\lambda_{t+1}$ according to eq. (7)
5: Update $z_{t+1}$ according to eq. (8)
6: end for
7: **Output:** $z_T$

where $\mathcal{L}(z, \lambda)$ is called the Lagrangian function and $\lambda$ is the dual variable. A simple approach to solving the minimax dual problem in eq. (1) is via the gradient descent and ascent method, which yields our algorithm of primal-dual bilevel optimizer (PDBO) (see Algorithm 1).

More specifically, the update of the dual variable $\lambda$ is via the gradient of Lagrangian w.r.t. $\lambda$ given by $\nabla_{\lambda}\mathcal{L}(z, \lambda) = \hat{h}(z)$, and the update of the primal variable $z$ is via the gradient of Lagrangian w.r.t. $z$ given by $\nabla_z\mathcal{L}(z, \lambda) = \nabla f(z) + \lambda\nabla h(z)$. Here, the differentiability of $\hat{h}(z)$ benefits from the constraint smoothing. In particular, suppose Assumption 1 holds. Then, it can be easily shown that $\hat{h}(z)$ is differentiable and $\nabla_x\hat{h}(x, y) = \nabla_x g(x, y) - \nabla_x g(x, \hat{y}^*(x))$, where $\hat{y}^*(x) = \arg \min_{y \in Y} g(x, y)$ is the unique minimal point of $\tilde{g}(x, y)$. Together with the fact that $\nabla_y\hat{h}(z) = \nabla_y g(z)$, we have
\[
\nabla\hat{h}(z) = (\nabla_x g(x, y) - \nabla_x g(x, \hat{y}^*(x)); \nabla_y g(x, y)). \tag{5}
\]

Since $\hat{y}^*(x)$ is the minimal point of the inner problem: $\min_{y \in Y} g(x_t, y) + \frac{\alpha}{2}\|y\|_2^2$, we conduct $N$ steps of projected gradient descent
\[
\hat{y}_{n+1} = \Pi_Y \left( \hat{y}_n - \frac{\alpha}{\rho + \beta} \left( \nabla_y g(x_t, \hat{y}_n) + \alpha \hat{y}_n \right) \right) \tag{6}
\]
as an estimate of $\hat{y}^*(x_t)$. Since the inner function $\tilde{g}(x, y)$ is $\alpha$-strongly convex w.r.t. $y$, updates in eq. (6) converge exponentially fast to $\hat{y}^*(x_t)$ w.r.t. $N$. Hence, with only a few steps, we can obtain a good estimate. With the output $\hat{y}_N$ of eq. (6) as the estimate of $\hat{y}^*(x_t)$, we conduct the gradient ascent and descent as follows:
\[
\lambda_{t+1} = \max \left\{ \lambda_t + \gamma \hat{h}(z_t) \right\}, \tag{7}
\]
\[
z_{t+1} = \Pi_Z \left( z_t - \beta \left( \nabla f(z_t) + \lambda_{t+1} \nabla\hat{h}(z_t) \right) \right), \tag{8}
\]
where $\hat{h}(z_t) = g(x_t, y_t) - \tilde{g}(x_t, \hat{y}_N)$ and $\nabla\hat{h}(z_t) = \nabla g(z_t) - (\nabla_x g(x_t, \hat{y}_N); \theta_d)$.

The convergence of the PDBO algorithm can be obtained via standard analysis for the primal-dual approach in [Daskalakis & Panageas, 2018; Jin et al., 2020; Lin et al., 2020]. However, since both $f(z)$ and $\hat{h}(z)$ are nonconvex in general, the solution of the dual problem eq. (1) serves only as an upper bound on the primal constrained problem eq. (3). More sophisticated design will be needed (as we will present in the next subsection) to have stronger guarantee for the constrained optimization.

In summary, PDBO features simple design and implementation, and solves bilevel problems with multiple inner minima with desirable solutions as we will show in our experiments in Section 3. In practice, such primal-dual algorithms are widely used for solving constrained nonconvex problems due to their simplicity and efficiency.
3.3 Proximal-PDBO Algorithm

In order to solve the constrained optimization problem eq. (3) (which is nonconvex optimization with a nonconvex constraint) with stronger convergence guarantee, we will adopt the proximal method Boob et al. (2019); Ma et al. (2020). The general idea is to iteratively solve a series of sub-problems, constructed by regularizing the objective and constrained functions into strongly convex functions. In this way, the algorithm is expected to converge to a stochastic $\epsilon$-KKT point (see Definition 2 in Section 4) of the primal problem in eq. (3).

By applying the proximal method, we obtain the Proximal-PDBO algorithm (see Algorithm 2) for solving the bilevel optimization problems formulated in eq. (3). At each iteration, the algorithm first constructs two proximal functions corresponding to the objective $f(z)$ and constraint $\tilde{h}(z)$ via regularizers. Since $f(z)$ is $\rho_f$ gradient Lipschitz as assumed in Assumption 2, the constructed function $\tilde{f}(z)$ is strongly convex. For the constraint $\tilde{h}(z)$, we next show that it inherits the gradient Lipschitz property from $g(z)$ below.

**Lemma 1.** Suppose that Assumptions 1, 2 hold. Then, $\nabla \tilde{h}(z)$ is Lipschitz continuous with the constant $\rho_h = \rho_g(2 + \rho_g/\alpha)$.

Following Lemma 4 the regularized function $\tilde{h}_k(z)$ also becomes strongly convex. Thus, $f_k(x)$ and $\tilde{h}_k(z)$ provide a new constrained optimization problem indexed by $(P_k)$ in Algorithm 2 with strongly convex objective and constraint, for which the strong duality holds immediately. It is thus equivalent to solving the dual problem of $(P_k)$, i.e., finding the saddle points of its Lagrangian given by

$$
\max_{\lambda \geq 0} \min_{z \in \mathcal{Z}} \mathcal{L}_k(z, \lambda) := f_k(z) + \lambda \tilde{h}_k(z).
$$

where $\lambda$ is the dual variable.

Then lines 5-11 in Algorithm 2 provides a solver for solving the problem in eq. (9) by the gradient descent and ascent algorithm. Similarly to PDBO, we first conduct $N$ steps of projected gradient descent obtain a good estimate $\hat{y}_N$ of $y^*(x)$. We then calculate the estimation of $\tilde{h}_k(z_t)$ and $\nabla \tilde{h}_k(z_t)$ using $\hat{y}_N$ as follows.

$$
\tilde{h}_k(z_t) = g(x_t, y_t) - \tilde{g}(x_t, \hat{y}_N) - \delta + \rho_h \|z_t - \tilde{z}_k\|^2_2,
$$

$$
\nabla \tilde{h}_k(z_t) = \nabla g(z_t) - \left( \begin{array}{c} \nabla_x \tilde{g}(x_t, \hat{y}_N) \\ 0_d \end{array} \right) + 2\rho_h (z_t - \tilde{z}_k).
$$

The gradient of the Lagrangian is immediately obtained through $\nabla_\lambda \mathcal{L}_k(z_t, \lambda_t) = \tilde{h}_k(z_t)$ and $\nabla_z \mathcal{L}_k(z_t, \lambda_{t+1}) = \nabla f_k(z_t) + \lambda_{t+1} \nabla \tilde{h}_k(z_t)$. The main step is to update the dual and primal variables $\lambda$ and $z$ alternatively. In particular, the dual variable is updated via projected accelerated gradient ascent as follows:

$$
\lambda_{t+1} = \Pi_{\Lambda} \left( \lambda_t + \frac{1}{\eta_t} \left((1 + \theta_t)\tilde{h}_k(z_t) - \theta_t \tilde{h}_k(z_{t-1}) \right) \right),
$$

where $1/\eta_t$ is the stepsize, $\theta_t$ is the weight of acceleration and $\Lambda$ is a bounded closed subset of $\mathbb{R}_{\geq 0}$ that contains all optimal dual variables. The primal variable $z$ is updated by the gradient descent with a stepsize $1/\tau_t$ as follows:

$$
z_{t+1} = \Pi_{\mathcal{Z}} \left( z_t - \frac{1}{\tau_t} \nabla_\lambda \mathcal{L}_k(z_t, \lambda_{t+1}) \right).
$$
Algorithm 2 Proximal-PDBO Algorithm

1: Input: Stepsizes \( \{\eta_t\} \) and \( \{\tau_t\} \), output weights \( \{\gamma_t\} \) and iteration numbers \( K \), and \( T \)
2: Set \( \tilde{z}_0 \) be any point inside \( Z \)
3: for \( k = 1, ..., K \) do
4:     Set the sub-problem
5:     \[
\min_{z \in Z} f_k(z) = f(z) + \rho_f \|z - \tilde{z}_{k-1}\|^2_2 \\
\text{s.t. } \tilde{h}_k(z) = \tilde{h}(z) + \rho_h \|z - \tilde{z}_{k-1}\|^2_2
\] (P_k)
6:     Internalize \( z_0 = z_{-1} = \tilde{z}_{k-1} \) and \( \lambda_0 = \lambda_{-1} = 0 \)
7:     for \( t = 0, 1, ..., T - 1 \) do
8:         Conduct projected gradient descent in eq. \( \text{(6)} \) for \( N \) times with any initial point \( \tilde{y}_0 \in Y \) to estimate \( \tilde{y}^*(x_t) \)
9:         Update \( \lambda_{t+1} \) according eq. \( \text{(10)} \)
10:    end for
11:    Set \( \tilde{z}_k = \frac{1}{T} \sum_{t=0}^{T-1} \gamma_t z_{t+1} \), with \( \Gamma_T = \sum_{t=0}^{T-1} \gamma_t \).
12: end for
13: Randomly pick \( \hat{k} \) from \( \{1, ..., K\} \)
14: Output: \( \hat{z}_k \)

4 Theoretical Results

4.1 Measure of Optimality

Since the constrained optimization problem eq. \( \text{(2)} \) is precisely equivalent to our original bilevel problem in eq. \( \text{(1)} \), we will define the criterion of the optimality guarantee for the problem in eq. \( \text{(2)} \). Since eq. \( \text{(2)} \) defines a nonconvex optimization problem with a nonconvex constraint, it is generally expected that the convergence will be expressed in terms of gradients. Since \( g^*(z) \) is only continuous and in general not differentiable, we need to find its subdifferential. We first define the subdifferential as follows.

Definition 1. Given a continuous function \( \omega(x) \) defined on \( X \subseteq \mathbb{R}^n \) and \( x \in X \), a vector \( v \in \mathbb{R}^n \) is a subdifferential of \( \omega(x) \) at \( x \) if and only if
\[
\lim_{x' \rightarrow x} \omega(x') - \omega(x) \geq \langle v, x' - x \rangle + o(\|x' - x\|_2).
\]
We denote \( \partial \omega(x) \) as the set of all subdifferentials at \( x \).

To characterize the subdifferential for \( g^*(x) \), we exploit its Lipschitz smoothness property, and further establish its following properties.

Lemma 2. Suppose Assumption \( 3 \) holds. Let \( G_{\tilde{x}}(x) = -g^*(x) + \frac{\omega(x - \tilde{x})}{\|x - \tilde{x}\|^2_2} \), where \( \tilde{x} \in X \) is a fixed point. Then \( G_{\tilde{x}}(x) \) is a convex function and \( \partial(-g^*)(...\tilde{x}) = \partial G_{\tilde{x}}(...\tilde{x}) \).

The above lemma ensures that although \( -g^*(x) \) is non-differentiable, it has well-defined subdifferentials. The subdifferential of \( h(z) := g(z) - g^*(z) \) w.r.t. \( x \) can then be obtained immediately by adding \( \nabla_x g(z) \) and \( \partial(-g^*)(...) \). Together with the fact that \( \nabla_y h(z) = \nabla_y g(z) \), the subdifferential \( \partial h(z) \) with respect to \( z \) is given by \( \partial h(z) = (\nabla_x g(z) + \partial(-g^*)(...) \nabla_y g(z))' \).

Assisted by the subdifferential \( \partial h(z) \) characterized above, we are ready to define the following first-order necessary condition of optimality for the nonconvex optimization problem with nonconvex constraint in eq. \( \text{(2)} \) [Boob et al. (2019); Ma et al. (2020)].
Definition 2 ((Stochastic) $\epsilon$-KKT point). Consider the constrained optimization problem in eq. (2). A point $\hat{z} \in Z$ is an $\epsilon$-KKT point if, there exist $z \in Z$ and $\lambda \geq 0$ such that $h(z) \leq 0$, $\|z - \hat{z}\|_2^2 \leq \epsilon$, $|\lambda h(z)| \leq \epsilon$, $|\lambda h(z)| \leq \epsilon$, and $\text{dist}(\nabla f(z) + \partial h(z) + \mathcal{N}(z; Z), 0) \leq \epsilon$, where $\mathcal{N}(z; Z)$ is the normal cone to $Z$ at $z$. For random $\hat{z} \in Z$, it is stochastic $\epsilon$-KKT points if there exist $z \in Z$ and $\lambda \geq 0$ such that the same requirements of $\epsilon$-KKT hold in expectation.

In this paper, we will take the above $\epsilon$-KKT condition as our convergence metric. It has been shown that the above KKT condition serves as the first-order necessary condition for the optimality guarantee for nonconvex optimization with nonconvex constraints under the MFCQ condition (see more details in Mangasarian & Fromovitz (1967)).

4.2 Convergence Guarantee

In this subsection, we establish the convergence guarantee for Proximal-PDBO, which does not follow directly from that for standard constrained nonconvex optimization [Boob et al. (2019); Ma et al. (2020)] due to the special challenges arising in bilevel problem formulations, as we discuss in the three steps of our proof below.

Our overall analysis consists of three steps, respectively corresponding to the following three propositions we prove, leading to the main theorem.

Step 1 characterizes the connection between the $\epsilon$-KKT point of the problem in eq. (2) (that is precisely equivalent to our original bilevel problem) and the $\epsilon$-KKT point of the problem in eq. (3) after smoothing and strict feasibility transformation (that is used for the design of Proximal-PDBO). We show that the difference between the two can be controlled by properly chosen the parameters $\alpha$ and $\delta$. The result is formalized as the following proposition.

Proposition 1. Suppose Assumptions 1 and 2 hold. If $z_k = (x_k, y_k)$ is an $\epsilon$-KKT point of the problem in eq. (3), it is an $\hat{\epsilon}$-KKT point of eq. (2) with $\hat{\epsilon} = \epsilon + O(\alpha) + O(\delta)$.

Proposition 1 indicates that the changes on the geometry of the constrained optimization have only mild impact on the convergent KKT point as long as $\alpha$ and $\delta$ are chosen at the level of $O(\epsilon)$.

Step 2 considers the sub-problems $(P_k)$ in Proximal-PDBO, which are constrained optimization with strongly convex objective and constraint. It is well-known that such a problem admits a unique global optimizer $z^*_k$ and optimal dual variable $\lambda^*_k$ for each $k$. Our following proposition shows that optimal dual variables $\lambda^*_k$ over all iterations $k \in \mathbb{N}$ have a uniform upper bound. Such an upper bound is critical to establish the convergence for the sub-problems as well as the final convergence for the overall algorithm for the constrained nonconvex optimization problem. We note that such a result was made as assumption in Boob et al. (2019).

Proposition 2. All sub-problems $(P_k)$ for $k \in \mathbb{N}$ during the execution of Proximal-PDBO have their optimal dual variable $\lambda^*_k$ satisfying a uniform upper bound, i.e., $\lambda^*_k \leq B \equiv L_f D_Z / \delta$ for all $k \in \mathbb{N}$.

Step 3 characterizes the convergence of solving the sub-problem $(P_k)$ defined in Proximal-PDBO. Our proof here is more challenging than the standard formulation studied in Boob et al. (2019); Ma et al. (2020) due to the nature of the bilevel optimization. Specifically, the constraint function here includes the minimal value $\hat{g}(x_t, y^*)$ of the inner function, where both its value and the minimal point will be estimated during the execution of algorithm, which will cause the gradients of both primal and dual variables to have bias errors. Our analysis will need to deal with such bias errors and characterize their impact on the convergence. The following proposition formalizes our result.
Proposition 3. Suppose Assumptions 1 and 2 hold. Let \( \gamma_t = \mathcal{O}(t) \), \( \eta_t = \mathcal{O}(t) \), \( \tau_t = \mathcal{O}(\frac{1}{t}) \) and \( \theta_t = \gamma_{t+1}/\gamma_t \), where the exact expressions can be found in Appendix D.1. Further let \( \Lambda = \{ \lambda \in \mathbb{R} : 0 \leq \lambda \leq B_\delta + 1 \} \) with \( B_\delta \) defined in Proposition 3. The optimality gap, constraint violation and distance from the optimal point of the output \( \hat{z}_k \) are all upper-bounded. More specifically, we have

\[
\begin{align*}
  f_k(\hat{z}_k) - f_k(z^*_k) &\leq \mathcal{O}\left( \frac{1}{\alpha^2\tau^2} \right) + \mathcal{O}\left( \frac{1}{\alpha^3\tau^3} \right), \\
  \max\{\hat{h}_k(z^*_k), \|\hat{z}_k - z^*_k\|^2\} &\leq \mathcal{O}\left( \frac{1}{\alpha^2\tau^2} \right) + \mathcal{O}\left( \frac{1}{\alpha^3\tau^3} \right).
\end{align*}
\]

We also note the following standard result on nonconvex constrained optimization proved in Boob et al. (2019) on the convergence of the outer-loop.

Lemma 3 (Theorem 3.17 Boob et al. (2019)). Suppose Assumptions 1 and 2 hold. And each subproblem is solved to \( \Delta \)-accuracy. Denote the global optimizer of \( (P_k) \) as \( z^*_k \), the optimality gap \( f_k(\hat{z}_k) - f_k(z^*_k) \), constraint violation \( \hat{h}_k(z^*_k) \), and distance to the solution \( \|\hat{z}_k - z^*_k\|^2 \) are upper-bounded by \( \Delta \). Then, the final output with a randomly chosen index is an stochastic \( \epsilon \)-KKT point of eq. (3), with \( \epsilon = \mathcal{O}\left( \frac{1}{\alpha^2\tau^2} \right) + \mathcal{O}\left( \frac{1}{\alpha^3\tau^3} \right) \).

Combining Propositions 1-3 and Lemma 3, we conclude the following convergence guarantee for our Proximal-PDBO.

Theorem 1. Suppose Assumptions 1 and 2 hold. Let the hyperparameters \( \Lambda, \gamma_t, \eta_t, \tau_t \) and \( \theta_t \) be the same as those in Proposition 3. Then, the output \( \hat{z}_k \) of Algorithm 2 with a randomly chosen index \( \hat{k} \) is a stochastic \( \epsilon \)-KKT point of eq. (2), where \( \epsilon \) is given by

\[
\epsilon = \mathcal{O}\left( \frac{1}{\alpha^2K^2} \right) + \mathcal{O}\left( \frac{1}{\alpha^3\tau^2} \right) + \mathcal{O}\left( \frac{1}{\alpha^4\tau^3} \right) + \mathcal{O}(\alpha) + \mathcal{O}(\delta).
\]

Theorem 1 indicates that the convergence of Proximal-PDBO is sublinear w.r.t. the number \( K \) of subproblem iterations and the number \( T \) of the Solver for solving each sub-problem, and linear w.r.t. the number \( N \) of iterations for obtaining the minimal value of the inner function.

We further note that Theorem 1 is the first finite-time convergence rate characterization for a bilevel optimizer that solves bilevel optimization problems with multiple inner minimal points.

5 Experiments

In this section, we first provide a numerical verification for our algorithm over a synthetic problem, and then apply it to hyperparameter optimization.

5.1 Numerical Verification

Consider the following bilevel optimization problem:

\[
\begin{align*}
\min_{x \in \mathbb{R}} & \quad f(x, y) := \frac{1}{2}\| (1, x) \|_2^2 - y \|_2^2 \\
\text{s.t.} & \quad y \in \arg \min_{y \in \mathbb{R}^2} \quad g(x, y) := \frac{1}{2}y_1^2 - xy_1,
\end{align*}
\]

where \( y \) is a vector in \( \mathbb{R}^2 \) and \( x \) is a scalar. It is not hard to analytically derive that the optimal solution of the problem in eq. (12) is \( (x^*, y^*) = (1, (1, 1)) \), which corresponds to the optimal objective values of \( f^* = 0 \) and \( g^* = -\frac{1}{2} \). For a given value of \( x \), the lower-level problem admits a unique minimal value \( g^*(x) = -\frac{1}{2}x \), which is attained at all points \( y = (x, a) \) with \( a \in \mathbb{R} \). Hence, the problem in eq. (12) violates the requirement of the
In fact, it can be analytically shown that standard AID and ITD approaches cannot solve the problem in existence of a single minimizer for the inner-problem, which is a strict requirement for most existing bilevel optimization methods, but still fall into our theoretical framework that allows multiple inner minimizers. In fact, it can be analytically shown that standard AID and ITD approaches cannot solve the problem in eq. 12 [Liu et al. 2020], which makes it both interesting and challenging.

We compare our algorithm PDBO with the following representative methods for bilevel optimization:

- **BigSAM + ITD** [Liu et al. 2020, Li et al. 2020]: uses sequential averaging to solve the inner problem and applies reverse mode automatic differentiation to compute hypergradient. This method is also designed to solve bilevel problems with multiple inner minima.

- **AID-FP** [Grazzi et al. 2020]: an approximate implicit differentiation approach with Hessian inversion using fixed point method. This method is guaranteed to converge when the lower-level problem admits a unique minimizer.

- **ITD-R** [Franceschi et al. 2017]: the standard iterative differentiation method for bilevel optimization, which differentiates through the unrolled inner gradient descent steps. We use its reverse mode implementation. This method is also guaranteed to converge when the lower level problem admits a unique minimizer.

For our algorithm PDBO, we set the learning rates $\lambda, \beta$ to be respectively 0.1, 0.2. For all compared
methods, we fix the inner and outer learning rates to respectively 0.5 and 0.2. We use $N = 5$ gradient descent steps to estimate the minimal value of the smoothed inner-objective and use the same number of iterations for all compared methods.

Figure 1 shows several evaluation metrics for the algorithms under comparison over different initialization points. It can be seen that our algorithm reaches the optimal solution at the fastest rate. Also as analytically proved in (Liu et al., 2020), several plots show that, with different initialization points, the classical AID and ITD methods cannot converge to the global optimal solution of the problem in eq. (12). In particular, algorithms AID-FP and ITD-R are both stuck in a bad local minima of the problem (fig. 1 (c), (d), (e), (h), and (i)). This is essentially due to the very restrictive unique minimizer assumption of these methods. When this fundamental requirement is not met, such approaches are not equipped with mechanisms to select among the multiple minimizers. Instead, our algorithm, which solves a constrained optimization problem, leverages the constraint set to guide the optimization process. Figure 2 further provides the optimization paths taken by the dual variable and the approximate values of the induced constraint $\tilde{h}$ for different initializations. The two plots show that the optimization terminates with a strictly positive dual variable and that the constraint is satisfied with equality, thus the slackness condition is satisfied. This also confirms that our algorithm PDBO did converge to a KKT point of the reformulated problem in eq. (3) for eq. (12).

Figure 2: Optimization path of dual variable and constraint values for different initializations.

5.2 Hyperparameter Optimization

The goal of hyperparameter optimization (HO) is to search for the set of hyperparameters that yield the optimal value of some model selection criterion (e.g., loss on unseen data). HO can be naturally expressed as a bilevel optimization problem, in which at the inner level one searches for the model parameters that achieve the lowest training loss for given hyperparameters. At the outer level, one optimizes the hyperparameters over a validation dataset. The problem can be mathematically formulated as follows

$$
\min_{\lambda, w} \mathcal{L}_{\text{val}}(\lambda, w) := \frac{1}{|D_{\text{val}}|} \sum_{\xi \in D_{\text{val}}} \mathcal{L}(\lambda, w; \xi)
$$

with

$$
w \in \arg \min_w \mathcal{L}_{\text{tr}}(\lambda, w) \text{ where }
\mathcal{L}_{\text{tr}}(\lambda, w) := \frac{1}{|D_{\text{tr}}|} \sum_{\zeta \in D_{\text{tr}}} \left( \mathcal{L}(\lambda, w; \zeta) + R(\lambda, w) \right)
$$

where $\mathcal{L}$ is a loss function, $R(w, \lambda)$ is a regularizer, and $D_{\text{tr}}$ and $D_{\text{val}}$ are respectively training and validation data.

Following (Franceschi et al., 2017; Grazzi et al., 2020a), we perform classification on the 20 Newsgroup dataset, where the classifier is modeled by an affine transformation and the cost function $\mathcal{L}$ is the cross-entropy loss. We set one $l_2$-regularization hyperparameter for each weight in $w$, so that $\lambda$ and $w$ have the same size. For our algorithm PDBO, we optimize the parameters and hyperparameters using gradient descent with a
fixed learning rate of $\beta = 100$. We set the learning rate for the dual variable to be 0.001. We use $N = 5$ gradient descent steps to estimate the minimal value of the smoothed inner-objective. For BigSAM+ITD, we set the averaging parameter to 0.5 and fix the inner and outer learning rates to be 100. For AID-FP and ITD-R, we use the suggested parameters in their implementations accompanying the paper [Grazzi et al., 2020a].

The evaluations of the algorithms under comparison on a hold-out test dataset is shown in Figure 3. It can be seen that our algorithm PDBO significantly improves over AID and ITD methods, and slightly outperforms BigSAM+ITD method with a much faster convergence speed.

6 Conclusion

In this paper, we investigated a bilevel optimization problem where the inner-level function has multiple minima. We reformulated such a problem into an equivalent single-level constrained optimization problem, based on which we designed two algorithms PDBO and Proximal-PDBO using primal-dual gradient descent and ascent method. Specifically, PDBO features a simple design and implementation, and Proximal-PDBO features a strong convergence guarantee that we can establish. We further conducted experiments to demonstrate the desirable performance of our algorithm. As future work, it is interesting to study bilevel problems with a nonconvex inner-level function, which can have multiple inner minima. While our current design can serve as a starting point, finding a good characterization of the set of inner minima can be challenging.

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Supplementary Materials

A Calculation of of $\nabla \tilde{h}(z)$ in eq. (5)

For completeness, we provide the steps to obtaining the form of $\nabla \tilde{h}(z)$ in eq. (5). For the ease of reading, we restate the result here. Suppose that Assumption 1 holds. Then the gradients $\nabla_x \tilde{h}(x, y)$ and $\nabla_y \tilde{h}(x, y)$ of function $\tilde{h}(x, y)$ take the following forms:

$$\nabla_x \tilde{h}(x, y) = \nabla_x g(x, y) - \nabla_x g(x, \tilde{y}^*(x)), \quad (13)$$
$$\nabla_y \tilde{h}(x, y) = \nabla_y g(x, y). \quad (14)$$

**Proof.** First, Equation (14) follows immediately. Hence, we prove only eq. (13). Recall the definition of $\tilde{h}(x, y)$:

$$\tilde{h}(x, y) = g(x, y) - \tilde{y}^*(x) - \delta,$$

where $\tilde{y}^*(x) = \tilde{g}(x, \tilde{y}^*(x))$ with $\tilde{y}^*(x) = \arg \min_y \tilde{g}(x, y) = g(x, y) + \frac{\alpha}{2}\|y\|^2$. Using the chain rule to compute the gradient with respect to $x$ of function $\tilde{h}(x, y) = g(x, y) - g(x, \tilde{y}^*(x)) - \frac{\alpha}{2}\|\tilde{y}^*(x)\|^2 - \delta$ yields:

$$\nabla_x \tilde{h}(x, y) = \nabla_x g(x, y) - \left[\nabla_x g(x, \tilde{y}^*(x)) + \frac{\partial \tilde{y}^*(x)}{\partial x} \nabla_y g(x, \tilde{y}^*(x))\right] - \frac{\partial g^*(x)}{\partial x} \tilde{y}^*(x)$$

$$= \nabla_x g(x, y) - \nabla_x g(x, \tilde{y}^*(x)) - \frac{\partial \tilde{y}^*(x)}{\partial x} \left[\nabla_y g(x, \tilde{y}^*(x)) + \alpha \tilde{y}^*(x)\right]. \quad (15)$$

The first order optimality condition ensures that $\nabla_y g(x, \tilde{y}^*(x)) + \alpha \tilde{y}^*(x) = 0$. Hence, we obtain the desired result:

$$\nabla_x \tilde{h}(x, y) = \nabla_x g(x, y) - \nabla_x g(x, \tilde{y}^*(x)). \quad (16)$$

B Proof of Lemma 1 in Section 3.3

Using eq. (5), we have:

$$\nabla \tilde{h}(z) = \begin{pmatrix} \nabla_x g(x, y) \\ \nabla_y g(x, y) \end{pmatrix} - \begin{pmatrix} \nabla_x g(x, \tilde{y}^*(x)) \\ 0_d \end{pmatrix} = \nabla g(z) - \begin{pmatrix} G_x \\ G_y \end{pmatrix}, \quad (17)$$

where $G_x = \nabla_x g(x, \tilde{y}^*(x))$ and $G_y = 0_d \in \mathbb{R}^d$ is a vector of all zeros. Taking derivative w.r.t. $z$ yields:

$$\nabla^2 \tilde{h}(z) = \nabla^2 g(z) - \begin{pmatrix} \frac{\partial G_x}{\partial x} & \frac{\partial G_x}{\partial y} \\ \frac{\partial G_y}{\partial x} & \frac{\partial G_y}{\partial y} \end{pmatrix}$$

$$= \nabla^2 g(z) - \begin{pmatrix} \frac{\partial \nabla_x g(x, \tilde{y}^*(x))}{\partial x} & 0_{p \times d} \\ 0_{d \times p} & 0_{d \times d} \end{pmatrix}. \quad (18)$$
where $0_{m \times n} \in \mathbb{R}^{m \times n}$ is a matrix of all zeros. We next upper-bound the 2-norm of the matrix $M$ defined above. We have:

$$\|M\|_2 = \left\| \begin{bmatrix} \frac{\partial g(x, \tilde{y}^*(x))}{\partial x} & 0_{p \times d} \\ 0_{d \times p} & 0_{d \times d} \end{bmatrix} \right\|_2 \leq \left\| \frac{\partial g(x, \tilde{y}^*(x))}{\partial x} \right\|_2,$$

where eq. (19) follows from the fact that for block matrix $C = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}$, we have $\|C\|_2 \leq \max\{\|A\|_2, \|B\|_2\}$. Further, using the chain rule we obtain

$$\frac{\partial g(x, \tilde{y}^*(x))}{\partial x} = \nabla^2 g(x, \tilde{y}^*(x)) + \frac{\partial \tilde{y}^*(x)}{\partial x} \nabla g(x, \tilde{y}^*(x)).$$

Thus, taking the norm yields

$$\left\| \frac{\partial g(x, \tilde{y}^*(x))}{\partial x} \right\|_2 \leq \left\| \nabla^2 g(x, \tilde{y}^*(x)) \right\|_2 + \left\| \frac{\partial \tilde{y}^*(x)}{\partial x} \right\|_2 \left\| \nabla g(x, \tilde{y}^*(x)) \right\|_2 \leq \rho_g + \rho_g \left\| \frac{\partial \tilde{y}^*(x)}{\partial x} \right\|_2.$$

Applying implicit differentiation w.r.t. $x$ to the optimality condition of $\tilde{y}^*(x)$ gives $\nabla^2 g(x, \tilde{y}^*(x)) + \alpha \frac{\partial \tilde{y}^*(x)}{\partial x} = 0$. This yields

$$\nabla^2 g(x, \tilde{y}^*(x)) + \alpha \frac{\partial \tilde{y}^*(x)}{\partial x} = 0$$

which further yields

$$\frac{\partial \tilde{y}^*(x)}{\partial x} = -\left[ \nabla^2 g(x, \tilde{y}^*(x)) + \alpha I \right]^{-1} \nabla g(x, \tilde{y}^*(x)).$$

Hence, we obtain

$$\left\| \frac{\partial \tilde{y}^*(x)}{\partial x} \right\|_2 \leq \left\| \left[ \nabla^2 g(x, \tilde{y}^*(x)) + \alpha I \right]^{-1} \right\|_2 \left\| \nabla g(x, \tilde{y}^*(x)) \right\|_2 \leq \frac{\rho_g}{\alpha},$$

where the last inequality follows from Assumptions 1 and 2. Hence, combining eq. (19), eq. (20), and eq. (21), we have

$$\|M\|_2 \leq \rho_g + \rho_g \frac{\rho_g}{\alpha},$$

which, in conjunction of eq. (18), yields

$$\|\nabla^2 h(z)\|_2 \leq \|\nabla^2 g(z)\|_2 + \|M\|_2 \leq \rho_g + \rho_g + \frac{\rho_g^2}{\alpha} = \rho_g \left( 2 + \frac{\rho_g}{\alpha} \right).$$

This completes the proof.

### C Proof of Lemma 2 in Section 4.1

Let $J(x) := -g^*(x) + \frac{\rho\|x - \bar{x}\|^2_2}{2}$, where $\bar{x}$ is an arbitrary point inside $\mathcal{X}$ and $g^*(x) = \min_{y \in \mathcal{Y}} g(x, y)$. We first prove that for any fixed $\rho \geq \rho_g$, we have $J(x)$ is a $\rho - \rho_g$ strongly convex function. Then, the claim $G_\varepsilon(x)$ is convex immediately follows. For any $x, \hat{x} \in \mathcal{X}$, and $0 \leq \lambda \leq 1$, we have

$$J(\lambda x + (1 - \lambda)\hat{x}) - \lambda J(x) - (1 - \lambda)J(\hat{x})$$
The above inequality implies that

\[ -g^*(\lambda x + (1 - \lambda)\bar{x}) + \frac{\rho}{2} ||\lambda x + (1 - \lambda)\bar{x}||^2 + \lambda g^*(x) - \frac{\lambda \rho}{2} ||x - \bar{x}||^2 + \lambda g^*(\bar{x}) - \frac{\lambda \rho}{2} ||\bar{x} - \bar{x}||^2 = \lambda [g^*(x) - g^*(\lambda x + (1 - \lambda)\bar{x})] + (1 - \lambda) [g^*(\bar{x}) - g^*(\lambda x + (1 - \lambda)\bar{x})] + \frac{\rho}{2} \left[ ||\lambda x + (1 - \lambda)\bar{x}||^2 - \lambda ||x||^2 - (1 - \lambda) ||\bar{x}||^2 \right]. \]

Hence, in this section, we will first provide proofs for the three propositions and then combine them together to prove Theorem 1.

D Proof of Theorem 1

The proof of Theorem 1 consists of three steps, respectively corresponding to the proofs of Propositions 1 to 3. Hence, in this section, we will first provide proofs for the three propositions and then combine them together to prove Theorem 1.
D.1 Proof of Proposition 1

**Proposition 4** (Formal Statement of Proposition 1). Suppose Assumptions 1 and 2 hold. If \( z_k = (x_k, y_k) \) is an \( \epsilon \)-KKT point of the reformulated problem in eq. (3) then there exists \( \bar{z} = (\bar{x}, \bar{y}) \) in a neighborhood of \( z_k \) (i.e., \( \| \bar{z} - z_k \|^2 \leq \epsilon \)) and \( \bar{\lambda} \geq 0 \) such that

\[
\begin{align*}
\bar{\lambda} \left[ g(\bar{x}, \bar{y}) - g^*(\bar{x}) \right] &\leq O(\epsilon) \\
\text{dist} \left( \nabla f(\bar{z}) + \bar{\lambda} \left[ \nabla_x g(\bar{x}, \bar{y}) - \nabla_g(\bar{x}, \bar{y}) \right] \right) + N(z; \mathcal{Z}), 0 \right)^2 &\leq O(\epsilon),
\end{align*}
\]

where \( y^*(\bar{x}) \) is a point in the set of minimal points, i.e., \( y^*(\bar{x}) \in \mathcal{S}_x \).

**Proof.** The definition of \( \epsilon \)-KKT point ensures that there exists \( \bar{z} = (\bar{x}, \bar{y}) \) with \( \| \bar{z} - z_k \|^2 \leq \epsilon \) and \( \bar{\lambda} \geq 0 \) such that

\[
|\bar{\lambda} h(\bar{z})| \leq \epsilon \quad (28)
\]

\[
\text{dist} \left( \nabla f(\bar{z}) + \bar{\lambda} \bar{\nabla} h(\bar{z}) + N(z; \mathcal{Z}), 0 \right)^2 \leq \epsilon. \quad (29)
\]

Replacing the expression of \( \bar{h}(\bar{z}) \) by its definition in eq. (28), we have:

\[
|\bar{\lambda} g(\bar{x}, \bar{y}) - \bar{\lambda} g^*(\bar{x}) - \bar{\lambda} \delta| \leq \epsilon
\]

\[
|\bar{\lambda} g(\bar{x}, \bar{y}) - \bar{\lambda} g^*(\bar{x})| - |\bar{\lambda} g^*(\bar{x}) - \bar{\lambda} \delta| \leq \epsilon
\]

where the last inequality follows from the triangle inequality. Therefore, we obtain

\[
\bar{\lambda} \left[ g(\bar{x}, \bar{y}) - g^*(\bar{x}) \right] \leq \bar{\lambda} |\bar{g}^*(\bar{x}) - g^*(\bar{x})| + \bar{\lambda} \delta + \epsilon
\]

\[
\leq D |\bar{g}^*(\bar{x}) - g^*(\bar{x})| + D \delta + \epsilon \quad (30)
\]

Further, we have

\[
|\bar{g}^*(\bar{x}) - g^*(\bar{x})| = |\min_y \bar{g}(\bar{x}, y) - \min_y g(\bar{x}, y)| \leq \max_y |\bar{g}(\bar{x}, y) - g(\bar{x}, y)| \leq \max_y \frac{\alpha}{2} \| y \|^2 = \frac{\alpha}{2} D^2. \quad (31)
\]

Combining eq. (30) and eq. (31) yields

\[
\bar{\lambda} \left[ g(\bar{x}, \bar{y}) - g^*(\bar{x}) \right] \leq \frac{\alpha D^2}{2} + D \delta + \epsilon.
\]

Hence, setting \( \alpha = O(\epsilon) \) and \( \delta = O(\epsilon) \), we obtain the first result of eq. (28)

\[
\bar{\lambda} \left[ g(\bar{x}, \bar{y}) - g^*(\bar{x}) \right] \leq O(\epsilon).
\]

Suppose \( v \in N(z; \mathcal{Z}) \) is the vector that attains the minimum of the following problem

\[
\min_{u \in N(\bar{z}; \mathcal{Z})} \| u + \nabla f(\bar{z}) + \bar{\lambda} \nabla h(\bar{z}) \|_2.
\]

In other words,

\[
\text{dist} \left( \nabla f(\bar{z}) + \bar{\lambda} \nabla h(\bar{z}) + N(z; \mathcal{Z}), 0 \right)^2 = \left\| v_x + \nabla_x f(\bar{x}, \bar{y}) + \bar{\lambda} \nabla_x h(\bar{x}, \bar{y}) \right\|^2 + \left\| v_y + \nabla_y f(\bar{x}, \bar{y}) + \bar{\lambda} \nabla_y h(\bar{x}, \bar{y}) \right\|^2.
\]
Hence eq. (29) implies
\[
\left\| v_x + \nabla_x f(\bar{x}, \bar{y}) + \bar{\lambda} \left[ \nabla_x g(\bar{x}, \bar{y}) - \nabla_x g(\bar{x}, \bar{y}^\star(\bar{x})) \right] \right\|^2 + \left\| v_y + \nabla_y f(\bar{x}, \bar{y}) + \bar{\lambda} \nabla_y g(\bar{x}, \bar{y}) \right\|^2 \leq \epsilon \tag{32}
\]

Let \( P_x = v_x + \nabla_x f(\bar{x}, \bar{y}) + \bar{\lambda} \left[ \nabla_x g(\bar{x}, \bar{y}) - \nabla_x g(\bar{x}, \bar{y}^\star(\bar{x})) \right] \). We have
\[
\left\| P_x \right\|^2 + \left\| P_y \right\|^2 = \left\| P_x \right\|^2 - \left\| \tilde{P}_x \right\|^2 + \left\| \tilde{P}_x \right\|^2 + \left\| P_y \right\|^2 \overset{(32)}{\leq} \left\| P_x \right\|^2 - \left\| \tilde{P}_x \right\|^2 + 2\epsilon. \tag{33}
\]

Also we have
\[
\left\| P_x \right\|^2 - \left\| \tilde{P}_x \right\|^2 = \left\langle P_x + \tilde{P}_x, P_x - \tilde{P}_x \right\rangle \leq \left\| P_x + \tilde{P}_x \right\| \left\| P_x - \tilde{P}_x \right\|
\]
\[
= \bar{\lambda} \left[ 2v_x + 2\nabla_x f(\bar{x}, \bar{y}) + 2\bar{\lambda} \nabla_x g(\bar{x}, \bar{y}) - \bar{\lambda} \nabla_x g(\bar{x}, \bar{y}^\star(\bar{x})) \right] \left\| \nabla_x g(\bar{x}, \bar{y}^\star(\bar{x})) - \nabla_x g(\bar{x}, \bar{y}^\star(\bar{x})) \right\|
\]
\[
\overset{(i)}{\leq} 6DL_g(L_f + 2DL_g) \| \bar{y}^\star(\bar{x}) - y^\star(\bar{x}) \|, \]

where \((i)\) follows because \( \left\| v_x \right\|_2 \leq 2 \| \nabla_x f(\bar{x}, \bar{y}) + \bar{\lambda} \nabla_x \hat{h}(\bar{x}, \bar{y}) \|_2 \), which can be easily proved by contradictory.

Hence, using the fact that \( \| \bar{y}^\star(\bar{x}) - y^\star(\bar{x}) \| \leq \mathcal{O}(\epsilon) \) for \( \alpha = \mathcal{O}(\epsilon) \), we obtain
\[
\left\| \| P_x \|^2 - \| \tilde{P}_x \|^2 \right\| \leq \mathcal{O}(\epsilon),
\]

which in conjunction of eq. (33) validates the second part of eq. (28)
\[
\left\| v_x + \nabla_x f(\bar{x}, \bar{y}) + \bar{\lambda} \left[ \nabla_x g(\bar{x}, \bar{y}) - \nabla_x g(\bar{x}, y^\star(\bar{x})) \right] \right\|^2 + \left\| v_y + \nabla_y f(\bar{x}, \bar{y}) + \bar{\lambda} \nabla_y g(\bar{x}, \bar{y}) \right\|^2 \leq \mathcal{O}(\epsilon).
\]

This is equivalent to
\[
\left\| v + \left( \nabla_x f(\bar{x}, \bar{y}) + \bar{\lambda} \left[ \nabla_x g(\bar{x}, \bar{y}) - \nabla_x g(\bar{x}, y^\star(\bar{x})) \right] \right) \right\|_2 \leq \mathcal{O}(\epsilon).
\]

Since \( v \in \mathcal{N}(\bar{x}, \mathcal{Z}) \), the above inequality completes the proof. \( \square \)

### D.2 Proof of Proposition 2

**Proposition 5** (Restatement of Proposition 2). For each subproblem \((P_k)\), there exists a unique global optimizer \( \hat{z}_k^\star \) and optimal dual variable \( \hat{\lambda}_k^\star \) such that \( \hat{\lambda}_k^\star \leq B_\delta := \frac{L_f D_\mathcal{Z}}{\delta} \).

**Proof.** For each sub-problem \((P_k)\), let \( \bar{z}_k = (\bar{x}_k, \bar{y}_k) \) with \( \bar{x}_k = (\bar{z}_{k-1})_x \) and \( \bar{y} = \arg \max_y g(\bar{x}_k, y) + \frac{\alpha \| y \|_2^2}{2} \). Then, we have \( \hat{h}_k(\bar{z}_k) = -\delta \), which is a strictly feasible point.

Define the function \( d(\lambda) = \min_{z \in \mathcal{Z}} \mathcal{L}_k(z, \lambda) \). Then, we have, for any \( \lambda \) and \( z \in \mathcal{Z} \),
\[
d(\lambda) \leq f_k(\bar{z}_k) + \hat{\lambda}_k(\bar{z}_k) = f_k(\bar{z}_k) - \delta \lambda, \tag{34}
\]

Moreover, it is known that constrained optimization with strongly convex objective and strongly convex constraints has no duality gap. Combining this with the fact that the optimal function value is bounded, we conclude that the optimal dual variable exists in \( \mathbb{R}_+ \). Taking \( \lambda = \lambda^\star \) in eq. (34) and using the fact that \( |d(\lambda^\star) - f_k(\bar{z}_k)| = |f_k(\bar{z}_k) - f_k(\bar{z}_k)| \leq L_f D_\mathcal{Z} \), we complete the proof. \( \square \)
D.3 Proof of Proposition 3

**Proposition 6** (Formal Statement of Proposition 3). Suppose Assumptions 1 and 2 hold. Let $\gamma_t = t + t_0 + 3$, $\eta_t = \eta(t + t_0 + 1)$, $\tau_t = \frac{4(L_\rho + 2\rho \eta D_z)^2}{\rho_T(t + 1)}$, $\theta_t = \frac{t + t_0 + 2}{t + t_0 + 3}$, where $t_0 = \frac{\rho_T + B \rho h}{\rho_T} + 1$, $B = B_3 + 1$ and $B_3$ defined in Proposition 3. We have

$$f_k(\bar{z}_k) - f_k(z^*_k) \leq \frac{2L_\rho BD_z}{\Gamma_T} \left( 1 - \frac{\alpha}{\rho_T + 2\alpha} \right)^N + \frac{(L_\rho + 2\rho h D_z)BD_z}{\Gamma_T} + (\rho h D_z + 3L_\rho)BD_z \left( 1 - \frac{\alpha}{\rho_T + 2\alpha} \right)^N + \frac{\gamma_0(\eta_0 - \rho f)}{\Gamma_T} z_k^* - z_0 \right|_2^2,$$

$\hat{h}_k(\bar{z}_k) \leq \frac{2L_\rho BD_z}{\Gamma_T} \left( 1 - \frac{\alpha}{\rho_T + 2\alpha} \right)^N + \frac{(L_\rho + 2\rho h D_z)BD_z}{\Gamma_T} + (\rho h D_z + 3L_\rho)BD_z \left( 1 - \frac{\alpha}{\rho_T + 2\alpha} \right)^N + \frac{\gamma_0(\eta_0 - \rho f)}{\Gamma_T} \left( \lambda_k^* - \lambda_0 \right)^2 + \gamma_0(\eta_0 - \rho f) \left| z_k^* - z_0 \right|^2,$

and

$$\left| \bar{z}_k - z_k^* \right|_2^2 \leq \frac{1}{\gamma_T} \left( \left( \eta_T - \frac{3(\rho f + B h)}{\rho_T} \right) \left( 4L_\rho BD_z \left( 1 - \frac{\alpha}{\rho_T + 2\alpha} \right)^N + 2(L_\rho + 2\rho h D_z)BD_z \right) \right) + \frac{1}{\gamma_T} \left( \left( \eta_T - \frac{3(\rho f + B h)}{\rho_T} \right) \left( \gamma_0(\eta_0 - \rho f) \left( \lambda_k^* - \lambda_0 \right)^2 + \gamma_0(\eta_0 - \rho f) \left| z_k^* - z_0 \right|^2 \right) \right) \frac{1}{\gamma_T} \left( \left( \eta_T - \frac{3(\rho f + B h)}{\rho_T} \right) (\rho h D_z + 3L_\rho)BD_z \left( 1 - \frac{\alpha}{\rho_T + 2\alpha} \right)^N \right).$$

**Proof.** We first define some notations that will be used later. Let $\hat{d}_t = (1 + \theta_t)\hat{h}_k(z_t) - \theta_t\hat{h}_k(z_t - 1)$, $d_t = (1 + \theta_t)\hat{h}_k(z_t) - \theta_t\hat{h}_k(z_t - 1)$, and $\xi_t = \hat{h}_k(z_t) - \hat{h}_k(z_t - 1)$. Further define the primal-dual gap function as

$$Q_k(w, \tilde{w}) := f_k(z) + \tilde{\lambda}h_k(z) - \left( \hat{f}_k(\tilde{z}) + \tilde{\lambda}h_k(\tilde{z}) \right),$$

where $w = (z, \lambda)$, $w = (\tilde{z}, \tilde{\lambda}) \in \mathcal{Z} \times \Lambda$ are primal-dual pairs.

Consider the update of $\lambda$ in eq. (10). Applying the following Lemma 4 with $v = -\hat{d}_t / \tau_t$, $S = \Lambda$, $x = \lambda_{t + 1}$, $x = \lambda_t$ and setting $\tilde{x} = \lambda$ be an arbitrary point inside $\Lambda$, we have

$$-(\lambda_{t + 1} - \lambda)\hat{d}_t \leq \frac{\eta_t}{2} \left( (\lambda - \lambda_t)^2 - (\lambda_{t + 1} - \lambda_t)^2 - (\lambda - \lambda_{t + 1})^2 \right). \tag{35}$$

**Lemma 4** (Lemma 3.5 [Lan, 2020]). Suppose $S$ is a convex and closed subset of $\mathbb{R}^n$, $x \in S$, and $v \in \mathbb{R}^n$. Define $\tilde{x} = \Pi_S (x - v)$. Then, for any $\tilde{x} \in S$, the following inequality holds.

$$\langle x, v \rangle + \frac{1}{2} \left\| \tilde{x} - \tilde{x} \right\|_2^2 + \frac{1}{2} \left\| x - \tilde{x} \right\|_2^2 \leq \frac{1}{2} \left\| x - \tilde{x} \right\|_2^2.$$

Similarly, consider the update of $z$ in eq. (11). Applying Lemma 4 with $v = \nabla_2 \mathcal{L}_k(z_t, \lambda_{t + 1}) / \eta_t$, $S = \mathcal{Z}$, $\tilde{x} = z_{t + 1}$, $x = z_t$ and let $\tilde{z} = z$ be an arbitrary point inside $\mathcal{Z}$, we obtain

$$\langle \nabla_2 \mathcal{L}_k(z_t, \lambda_{t + 1}), z_{t + 1} - z \rangle \leq \frac{\eta_t}{2} \left( (z - z_t)^2 - (z_{t + 1} - z_t)^2 - (z - z_{t + 1})^2 \right). \tag{36}$$

Recall that $f_k(z)$ and $\hat{h}_k(z)$ are $3\rho_f$- and $3\rho_h$-gradient Lipschitz. This implies

$$\langle \nabla f_k(z_t), z_{t + 1} - z \rangle \geq f_k(z_{t + 1}) - f_k(z_t) - \frac{3\rho_f \left\| z_t - z_{t + 1} \right\|_2^2}{2}, \tag{37}$$
\[(\nabla \tilde{h}_k(z_t), z_{t+1} - z_t) \geq \tilde{h}_k(z_{t+1}) - \tilde{h}_k(z_t) - \frac{3\rho_h}{2} z_t - z_{t+1}^2.\] (38)

Moreover, recall that \(f_k(z)\) and \(\tilde{h}_k(z)\) are \(\rho_f\) and \(\rho_h\) strongly convex functions. These two properties yield
\[
\langle \nabla f_k(z_t), z_t - z \rangle \geq f_k(z_t) - f_k(z) + \frac{\rho_f}{2} \|z - z_t\|^2, \tag{39}
\]
\[
\langle \nabla \tilde{h}(z_t), z_t - z \rangle \geq \tilde{h}(z_t) - \tilde{h}(z) + \frac{\rho_h}{2} \|z - z_t\|^2. \tag{40}
\]

Consider the exact gradient of Lagrangian with respect to the primal variable, we have
\[
\langle \nabla \mathcal{L}(z_t, \lambda_{t+1}), z_{t+1} - z \rangle = \langle \nabla f_k(z_t) + \lambda_{t+1} \nabla \hat{h}_k(z_t), z_{t+1} - z_t \rangle
= \langle \nabla f_k(z_t), z_{t+1} - z \rangle + \langle \nabla f_k(z_t), z - z_t \rangle + \lambda_{t+1}(\nabla \hat{h}_k(z_t), z_{t+1} - z) + \lambda_{t+1}(\nabla \hat{h}_k(z_t), z - z_t)
\geq f_k(z_{t+1}) - f_k(z) + \lambda_{t+1}(\hat{h}(z_{t+1}) - \hat{h}(z_t)) - \frac{3}{2}(\rho_f + \lambda_{t+1} \rho_h) \|z_{t+1} - z_t\|^2 + \frac{\rho_h}{2} \|z - z_t\|^2, \tag{41}
\]
where (i) follows from combining eqs. (37) to (40).

Combining eqs. (39) and (41) yields
\[
f_k(z_{t+1}) - f_k(z) \leq \langle \nabla \mathcal{L}(z_t, \lambda_{t+1}), z_{t+1} - z \rangle + \lambda_{t+1}(\hat{h}(z) - \hat{h}(z_{t+1}))
+ \frac{\eta_t}{2} \left(\frac{\rho_f}{2} + \lambda_{t+1} \rho_h\right) \|z - z_t\|^2 - \frac{\eta_t}{2} \left(\frac{\rho_h}{2} \|z - z_t\|^2 - \frac{\eta_t}{2} \|z - z_{t+1}\|^2\right). \tag{42}
\]

Recall the definition of \(\xi_t = \hat{h}(z_t) - \hat{h}(z_{t-1})\). Substituting it into eq. (35) yields
\[
0 \leq -\left(\lambda - \lambda_{t+1}\right) \hat{h}(z_{t+1}) - \left(\lambda_{t+1} - \lambda\right) \xi_{t+1} + \theta_t(\lambda_{t+1} - \lambda) \xi_t + \frac{\tau_t}{2} ((\lambda - \lambda_t)^2 - (\lambda_{t+1} - \lambda_t)^2 - (\lambda - \lambda_{t+1})^2). \tag{43}
\]

Let \(w = (z, \lambda)\) and \(w_{t+1} = (z_{t+1}, \lambda_{t+1})\). By the definition of the primal-dual gap function, we have
\[
Q(w_{t+1}, w) = f_k(z_{t+1}) + \lambda_{t+1} \hat{h}(z_{t+1}) - f_k(z) - \lambda_t \hat{h}(z)
\leq \langle \nabla \mathcal{L}(z_t, \lambda_{t+1}), z_{t+1} - z \rangle + \lambda_{t+1}(\hat{h}(z_{t+1}) - \hat{h}(z_t))
+ \frac{\eta_t}{2} \left(\frac{\rho_f}{2} + \lambda_{t+1} \rho_h\right) \|z - z_t\|^2 - \frac{\eta_t}{2} \left(\frac{\rho_h}{2} \|z - z_t\|^2 - \frac{\eta_t}{2} \|z - z_{t+1}\|^2\right). \tag{44}
\]
where (i) follows from eq. (42) and (ii) follows from eq. (43) and \(0 \leq \lambda_{t+1} \leq B\).

Now we proceed with \(|\hat{h}(z_t) - \hat{h}(z)|\).
\[
|\hat{h}(z_t) - \hat{h}(z)| = |g(x_t, \tilde{y}^*_t) - g(x_t, \tilde{y}^*_t)| \leq 2L_g \|\tilde{y}^*_t - \tilde{y}^*_t\| \leq L_g D_Z \left(1 - \frac{\alpha}{\rho_h + 2\alpha}\right)^N, \tag{45}
\]
where (i) follows from Assumption (2) and (ii) follows from the following Lemma (5) and \(\|\tilde{y}_0 - \tilde{y}^*(x_t)\| \leq D_Z\).
Lemma 5 (Theorem 2.2.14 [Nesterov et al. (2018)]). Suppose Assumptions 1 and 2 hold. Consider line 7 in Algorithm 2. Define \( \hat{y}^*(x_t) := \arg \min_{y \in Y} g(x_t, y) + \frac{\alpha}{2} \| y \|^2_2 \). We have
\[
\| \hat{y}^*(x_t) - y^*(x_t) \|_2 = \| \hat{y}_N - \hat{y}^*(x_t) \|_2 \leq \left( 1 - \frac{\alpha}{\rho_y + 2\alpha} \right)^N \| \hat{y}_0 - \hat{y}^*(x_t) \|_2.
\]
The following inequality follows immediately from the above eq. (45).
\[
(\lambda - \lambda_{t+1})(\tilde{h}_k(z_t) - \hat{h}_k(z_t)) \leq |\lambda - \lambda_{t+1}| \| \tilde{h}_k(z_t) - \hat{h}_k(z_t) \| \leq L_g B D_Z \left( 1 - \frac{\alpha}{\rho_y + 2\alpha} \right)^N.
\]
By the definitions of \( \nabla \mathcal{L}_k(z_t, \lambda_{t+1}) \) and \( \nabla \mathcal{L}_k(z_t, \lambda_{t+1}) \), we have
\[
\| \nabla \mathcal{L}_k(z_t, \lambda_{t+1}) - \nabla \mathcal{L}_k(z_t, \lambda_{t+1}) \|_2 \leq \lambda_{t+1} \| \nabla g_k(x_t, \hat{y}_t^*) - g_k(x_t, y^*_t) \|_2 + \lambda_{t+1} \rho_g \| \hat{y}_t^* - y^*_t \|_2 \leq B \rho_g D_Z \left( 1 - \frac{\alpha}{\rho_y + 2\alpha} \right)^N,
\]
where (i) follows from Assumption 2 and (ii) follows from Lemma 5 and because \( \lambda_{t+1} \leq B \) and \( \| \hat{y}_0 - \hat{y}^*(x_t) \|_2 \leq D_Z \).
By Cauchy-Schwartz inequality and eq. (47), we have
\[
\langle \nabla \mathcal{L}_k(z_t, \lambda_{t+1}) - \nabla \mathcal{L}_k(z_t, \lambda_{t+1}), z_{t+1} - z \rangle \leq \| \nabla \mathcal{L}_k(z_t, \lambda_{t+1}) - \nabla \mathcal{L}_k(z_t, \lambda_{t+1}) \|_2 \| z_{t+1} - z \|_2 \leq B \rho_g D_Z^2 \left( 1 - \frac{\alpha}{\rho_y + 2\alpha} \right)^N.
\]
By the definition of \( \xi_t \), we have
\[
\theta_t(\lambda_{t+1} - \lambda_t) \xi_t = \theta_t(\lambda_{t+1} - \lambda_t)(\hat{h}_k(z_t) - \tilde{h}_k(z_{t-1})) = \theta_t(\lambda_{t+1} - \lambda_t)(\hat{h}_k(z_t) - \tilde{h}_k(z_{t-1}) + \tilde{h}_k(z_{t-1}) + \hat{h}_k(z_{t-1} - \tilde{h}_k(z_{t-1}))) \leq \theta_t |\lambda_{t+1} - \lambda_t| \left( |\hat{h}_k(z_t) - \tilde{h}_k(z_{t-1})| + |\tilde{h}_k(z_{t-1}) - \hat{h}_k(z_{t-1})| + |\hat{h}_k(z_{t-1}) - \tilde{h}_k(z_{t-1})| \right)
\leq (i) \leq (\lambda_{t+1} - \lambda_t) \left( 2 L_g D_Z \left( 1 - \frac{\alpha}{\rho_y + 2\alpha} \right)^N + (L_g + 2 \rho_D D_Z) \| z_t - z_{t-1} \|_2 \right)
\leq (ii) \leq 2 B L g D_Z \left( 1 - \frac{\alpha}{\rho_y + 2\alpha} \right)^N + (L_g + 2 \rho_D D_Z) \| \lambda_{t+1} - \lambda_t \|_2 \| z_t - z_{t-1} \|_2
\leq (iii) \leq 2 B L g D_Z \left( 1 - \frac{\alpha}{\rho_y + 2\alpha} \right)^N + \frac{\eta_t}{2} (\lambda_{t+1} - \lambda_t)^2 + \frac{(L_g + 2 \rho_D D_Z)^2}{2 \tau_t} \| z_t - z_{t-1} \|_2^2.
\]
where (i) follows from eq. (45), \( \theta_t \leq 1 \), and \( \hat{h}_k(z) \) is \( L_g + 2 \rho_D D_Z \) Lipschitz continuous, (ii) follows from 0 \( \leq \lambda_t, \lambda_{t+1} \leq B \), and (iii) follows from Young’s inequality.
Substituting eqs. (46), (48) and (49) into eq. (44) yields
\[
Q(w_{t+1}, w) \leq -(\lambda_{t+1} - \lambda) \xi_{t+1} + \theta_t(\lambda_t - \lambda) \xi_t + (\rho_D D_Z + 3 L_g) B D_Z \left( 1 - \frac{\alpha}{\rho_y + 2\alpha} \right)^N
+ \frac{\eta_t}{2} \left( (\lambda - \lambda_t)^2 + (\lambda - \lambda_{t+1})^2 \right) + \frac{\eta_t - \rho_f}{2} \| z - z_t \|_2 - \frac{\eta_t}{2} \| z - z_{t+1} \|_2^2
+ \frac{(L_g + 2 \rho_D D_Z)^2}{2 \tau_t} \| z_t - z_{t-1} \|_2^2 - \frac{\eta_t - 3 \rho_f + B \rho_h}{2} \| z - z_{t+1} \|_2^2.
\]
Recall that $\gamma_t, \theta_t, \eta_t$, and $\tau_t$ are set to satisfy $\gamma_{t+1} \theta_{t+1} = \gamma_t, \gamma_t \tau_t \geq \gamma_{t+1} \tau_{t+1}$ and 
\[
\gamma_t(\rho_f + B \rho h) - \eta_t + \frac{2 \gamma_{t+1} (L_g + 2 \rho_h D \xi)}{\tau_{t+1}} \leq 0.
\]

Multiplying $\gamma_t$ on both sides of eq. (50) and telescoping from $t = 0, 1, \ldots T - 1$ yield
\[
\sum_{t=0}^{T-1} \gamma_t Q(w_{t+1}, w) \leq -\gamma_{T-1}(\lambda_T - \lambda) \xi_T + (\rho_g D_g + 3 L_g) BD \xi \left( 1 - \frac{\alpha}{\rho_g + 2\alpha} \right)^N \sum_{t=0}^{T-1} \gamma_t \\
+ \frac{\gamma_0 \tau_0}{2} (\lambda - \lambda_0)^2 + \frac{\gamma_0 (\eta_0 - \rho_f)}{2} \|z - z_0\|^2 - \frac{\gamma_{T-1}(\eta_{T-1} - 3(\rho_f + B \rho h))}{2} \|z - z_T\|^2.
\]

Divide both sides of the above inequality by $\Gamma_T = \sum_{t=0}^{T-1} \gamma_t$. We obtain
\[
\frac{1}{\Gamma_T} \sum_{t=0}^{T-1} \gamma_t Q(w_{t+1}, w) \leq -\frac{\gamma_{T-1}(\lambda_T - \lambda) \xi_T}{\Gamma_T} + (\rho_g D_g + 3 L_g) BD \xi \left( 1 - \frac{\alpha}{\rho_g + 2\alpha} \right)^N \\
+ \frac{\gamma_0 \tau_0}{2T} (\lambda - \lambda_0)^2 + \frac{\gamma_0 (\eta_0 - \rho_f)}{2T} \|z - z_0\|^2 - \frac{\gamma_{T-1}(\eta_{T-1} - 3(\rho_f + B \rho h))}{2T} \|z - z_T\|^2.
\]

Similarly to the steps in eq. (49), we have
\[
|\lambda_T - \lambda| \xi_T \leq |\lambda_T - \lambda| \left( 2 L_g D \xi \left( 1 - \frac{\alpha}{\rho_g + 2\alpha} \right)^N + (L_g + 2 \rho_h D \xi) \|z_T - z_{T-1}\|^2 \right) \\
\leq 2 L_g BD \xi \left( 1 - \frac{\alpha}{\rho_g + 2\alpha} \right)^N + (L_g + 2 \rho_h D \xi) BD \xi.
\]

Define $\hat{w}_k := \frac{1}{\Gamma_T} \sum_{t=0}^{T-1} \gamma_t w_{t+1}$. Noting that $Q(\cdot, w)$ is a convex function and substituting the above inequality into eq. (51) yield
\[
Q(\hat{w}_k, w) \leq \frac{1}{\Gamma_T} \sum_{t=0}^{T-1} \gamma_t Q(w_{t+1}, w) \leq 2 L_g BD \xi \left( 1 - \frac{\alpha}{\rho_g + 2\alpha} \right)^N + (L_g + 2 \rho_h D \xi) BD \xi \left( 1 - \frac{\alpha}{\rho_g + 2\alpha} \right)^N \\
+ \frac{\gamma_0 \tau_0}{2T} (\lambda - \lambda_0)^2 + \frac{\gamma_0 (\eta_0 - \rho_f)}{2T} \|z - z_0\|^2 - \frac{\gamma_{T-1}(\eta_{T-1} - 3(\rho_f + B \rho h))}{2T} \|z - z_T\|^2.
\]

Let $w = (z^*_k, 0)$. Then, we have
\[
Q(\hat{w}_k, w) = f_k(\hat{z}_k) - f_k(z^*_k) - \lambda_\hat{h}k(z^*_k) \geq f_k(\hat{z}_k) - f_k(z^*_k),
\]
where (i) follows from the fact $\hat{h}k(z_T^*) \leq 0$ and $\lambda_\hat{h} = \frac{1}{\Gamma_T} \sum_{t=0}^{T-1} \gamma_t \lambda_{t+1} \geq 0$.

Substituting the above inequality into eq. (52) yields
\[
f_k(\hat{z}_k) - f_k(z^*_k) \leq 2 L_g BD \xi \left( 1 - \frac{\alpha}{\rho_g + 2\alpha} \right)^N + (L_g + 2 \rho_h D \xi) BD \xi \left( 1 - \frac{\alpha}{\rho_g + 2\alpha} \right)^N \\
+ (\rho_g D_g + 3 L_g) BD \xi \left( 1 - \frac{\alpha}{\rho_g + 2\alpha} \right)^N + \frac{\gamma_0 (\eta_0 - \rho_f)}{2T} \|z^*_k - z_0\|^2.
\]

Recall that $(z_k^*, \lambda_k^*)$ is a Nash equilibrium of $L_k(z, \lambda)$, we have
\[
L_k(\hat{z}_k, \lambda_k) \geq L_k(z^*_k, \lambda^*_k) \iff f_k(\hat{z}_k) + \lambda_k^* \hat{h}_k(\hat{z}_k) - f_k(z^*_k) \geq 0
\]

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Let \( w = (z_k^*, (\lambda_k^* + 1)I(\hat{h}_k(\hat{z}_k))) \), where \( I(x) = 0 \) if \( x \leq 0 \) and \( I(x) = 1 \) otherwise. If \( \hat{h}_k(\hat{z}_k) \leq 0 \), the constraint is satisfied. If \( \hat{h}_k(\hat{z}_k) > 0 \), we have

\[
Q(\hat{w}_k, w) = f_k(\hat{z}_k) + (\lambda_k^* + 1)\hat{h}_k(\hat{z}_k) - f_k(z_k^*) - \lambda_k^*\hat{h}_k(\hat{z}_k).
\]  

(55)

Recall that \((z_k^*, \lambda_k^*)\) satisfies the KKT condition of \((P_k)\), i.e. \( \lambda_k^*\hat{h}_k(z_k^*) = 0 \). Equations (52), (54) and (55) together yield,

\[
\hat{h}_k(\hat{z}_k) = Q(\hat{w}_k, w) - (f_k(\hat{z}_k) + \lambda_k^*\hat{h}_k(\hat{z}_k) - f_k(z_k^*)) \leq Q(\hat{w}_k, w)
\]

\[ \leq \frac{2L_gBD_Z}{\gamma_T} \left( 1 - \frac{\alpha}{\rho_{\gamma} + 2\alpha} \right)^N + \frac{(L_g + 2\rho_D Z)BD_Z}{\gamma_T} + (\rho_g D_Z + 3L_g)BD_Z \left( 1 - \frac{\alpha}{\rho_{\gamma} + 2\alpha} \right)^N \]

\[ + \frac{\gamma_0 \tau_0 (\lambda_k^* + 1)^2}{2\gamma_T} + \frac{\gamma_0(\eta_0 - \rho_f)}{2\gamma_T}\|\hat{z}_k\|^2. \]

(56)

Finally, taking \( w^* = (z_k^*, \lambda_k^*) \) in eq. (52), noticing the fact \( Q(\cdot, w^*) \geq 0 \) for all \( w \), and rearranging the terms, we have

\[
\|\hat{z}_k - z_k^*\|^2 \leq \frac{1}{\gamma_{T-1}(\eta_{T-1} - 3(\rho_f + B\rho_h))} \left( 4L_gBD_Z \left( 1 - \frac{\alpha}{\rho_{\gamma} + 2\alpha} \right)^N + 2(L_g + 2\rho_D D_Z)BD_Z \right)
\]

\[ + \frac{1}{\gamma_{T-1}(\eta_{T-1} - 3(\rho_f + B\rho_h))} \left( \gamma_0 \tau_0 (\lambda_k^* - \lambda_0)^2 + \gamma_0(\eta_0 - \rho_f)\|z_k^* - z_0\|^2 \right)
\]

\[ + \frac{\rho_D D_Z + 3L_g)BD_Z \left( 1 - \frac{\alpha}{\rho_{\gamma} + 2\alpha} \right)^N. \]

(57)

\[ \square \]

D.4 Proof of Theorem 1

The proof of Theorem 1 follows from applying Propositions 1 to 3 and Lemma 3. First, Proposition 2 ensures the assumption of Lemma 3 holds.

Now applying Proposition 3, we have for every \( k = 1, 2, \ldots, K \), \( \hat{z}_k \) is a \( \Delta \)-accurate solution of sub-problem \((P_k)\) with

\[
\Delta = \mathcal{O} \left( \frac{1}{\alpha^3 \delta^3 T^2} \right) + \mathcal{O} \left( \frac{1}{\alpha \delta e N} \right).
\]

(58)

Then, applying Lemma 3 with \( \Delta \) specified in eq. (58), we have that the output \( \hat{z}_k \) is \( \hat{\epsilon} \)-KKT point of eq. (2) with \( \hat{\epsilon} \) equals to

\[
\epsilon = \mathcal{O} \left( \frac{1}{\alpha^2 \delta^2 K} \right) + \mathcal{O} \left( \frac{1}{\alpha^4 \delta^5 T^2} \right) + \mathcal{O} \left( \frac{1}{\alpha^2 \delta^3 e^{-N}} \right).
\]

(59)

Finally, applying Proposition 1 with \( \epsilon \) specified in eq. (59), we conclude that \( \hat{z}_k \) is an \( \epsilon \)-KKT point of eq. (2) with \( \epsilon \) specified below.

\[
\epsilon = \mathcal{O} \left( \frac{1}{\alpha^2 \delta^2 K} \right) + \mathcal{O} \left( \frac{1}{\alpha^4 \delta^5 T^2} \right) + \mathcal{O} \left( \frac{1}{\alpha \delta^2 e^{-N}} \right) + \mathcal{O}(\alpha) + \mathcal{O}(\delta).
\]

This completes the proof.

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