Functional Constrained Optimization for Risk Aversion and Sparsity Control

Yi Cheng, Guanghui Lan, H. Edwin Romeijn*

H. Milton Stewart School of Industrial and Systems Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, cheng.yi@gatech.edu, george.lan@isye.gatech.edu, edwin.romeijn@isye.gatech.edu

Risk and sparsity requirements often need to be enforced simultaneously in many applications, e.g., in portfolio optimization, assortment planning, and treatment planning. Properly balancing these potentially conflicting requirements entails the formulation of functional constrained optimization with either convex or nonconvex objectives. In this paper, we focus on projection-free methods that can generate a sparse trajectory for solving these challenging functional constrained optimization problems. Specifically, for the convex setting, we propose a Level Conditional Gradient (LCG) method, which leverages a level-set framework to update the approximation of the optimal value and an inner conditional gradient oracle (CGO) for solving mini-max subproblems. We show that the method achieves $O\left(\frac{1}{\epsilon^2 \log \frac{1}{\epsilon}}\right)$ iteration complexity for solving both smooth and nonsmooth cases without dependency on a possibly large size of optimal dual Lagrange multiplier.

For the nonconvex setting, we introduce the Level Inexact Proximal Point (IPP-LCG) method and the Direct Nonconvex Conditional Gradient (DNCG) method. The first approach taps into the advantage of LCG by transforming the problem into a series of convex subproblems and exhibits an $O\left(\frac{1}{\epsilon^3 \log \frac{1}{\epsilon}}\right)$ iteration complexity for finding an $(\epsilon, \epsilon)$-KKT point. The DNCG is the first single-loop projection-free method, with iteration complexity bounded by $O\left(\frac{1}{\epsilon^4}\right)$ for computing a so-called $\epsilon$-Wolfe point. We demonstrate the effectiveness of LCG, IPP-LCG and DNCG by devising formulations and conducting numerical experiments on two risk averse sparse optimization applications: a portfolio selection problem with and without cardinality requirement, and a radiation therapy planning problem in the healthcare area.

1. Introduction

Making decisions from the point of view of risk aversion arises widely in many important applications, such as financial engineering (Föllmer and Schied 2002, Hull 2006, McNeil et al. 2015), supply chain management (March and Shapira 1987, Tomlin 2006) and power system operations (Carrión et al. 2007, Conejo et al. 2010). Risk aversion optimization provides a framework for managing fluctuations of specific realizations of the underlying random process, which is critically important especially when tail-probability event relates to the failure or catastrophic disruption of the system being optimized. For example, consider a portfolio selection problem of maximizing the expected return, the optimal strategy suggests directing all investment to the asset with the highest

* Cheng and Lan were partially supported by the NSF Grant CCF 1909298 and the NSF AI Institute grant NSF-2112533.
expected return, which may result in losing all or a large amount of the invested principal when the realized return of the asset is very low. Furthermore, in many applications of risk averse optimization, solution sparsity is desirable. This happens, for example, in portfolio selection when the number of selected assets is capped and in assortment planning when number of items in the assortment is limited. In addition, sparse solutions are often easier to store and actuate. For instance, in signal processing, sparse approximate solutions are sought after as they can be processed, stored and transmitted in an efficient fashion. As such, sparse optimization finds rich applications in compressed sensing (Figueiredo et al. 2007, Goldfarb et al. 2013), sparse learning (Tibshirani 1996, Blumensath and Davies 2008) and matrix completion (Candes et al. 2008, Cai et al. 2010).

In risk averse optimization, risk aversion is often manifested by risk measures such as Value-at-Risk (VaR) (Artzner et al. 1999) and Conditional Value-at-Risk (CVaR) (Rockafellar et al. 2000, Rockafellar and Uryasev 2002). To be specific, given a probability level \( \alpha \in (0, 1) \), VaR is defined as the left-side \( \alpha \)-quantile of a random variable while CVaR represents the expected value of the \( \alpha \)-quantile distribution and is a convex approximation of (VaR). Other widely adopted risk measures include entropic, mean-variance and mean-upper-semideviation risk measure (see Section 6, Shapiro et al. 2021), to name a few. In some applications (e.g. distributionally robust optimization), risk is also coined by probabilistic form (e.g. chance constraints). Optimizing over the risk measure, either as a constraint or an objective, is commonly used to construct risk averse policies. While convex risk measures result in tractable formulations, nonconvex risk measures such as Value-at-Risk or chance constraints are more appropriate to model and control the risk in some situation.

In sparse optimization, a sparse formulation often aims to find an approximate minimizer (maximizer) that follows the cardinality constraint modeled by \( \ell_0 \)-norm, i.e. the number of nonzeros within the solution is less than a given level. As a convex surrogate of the \( \ell_0 \)-norm, \( \ell_1 \)-norm is also shown to promote solution sparsity. In many scenarios when solution structure can not be attained by the simple sparsity formulation as mentioned above, group sparsity (e.g., sum of a group of \( \ell_p \) norm, \( p > 0 \)) is used to select or deselect the elements in the decision vector at the group level. On top of that, nuclear norm \( \|X\|_* \) (sum of singular values) is often exerted to induce low rank structure, such as in matrix completion. Similar to risk aversion, these aforementioned sparsity requirements can be incorporated either as a regularization term in the objective or a constraint in defining the feasible set.

Risk averse optimization and sparse optimization have been studied separately in most existing literature. These requirements are sometimes conflicting, for example, a diversified selection of portfolio can reduce the risk but may lead to the violation of the cardinality constraint on the number of assets. Therefore, joint consideration of risk aversion and sparsity appears to be
very important in a wide range of applications, e.g., cardinality-constrained assortment planning, cardinality-constrained portfolio selection, power grid optimization and radiation therapy planning. This motivate us to consider a class of functional constrained optimization problems that can be used to model jointly sparsity requirement and risk aversion. In particular, the main problem of interest in this paper is given in the form of

\[
\begin{align*}
    f^* := & \min f(x) \\
    \text{s.t. } & h_i(x) \leq 0, \ i = 1, \cdots, m, \\
    & x \in X,
\end{align*}
\]  

(1.1)

where \( f : X \to \mathbb{R} \) is proper lower semicontinuous function (not necessarily convex), \( h := (h_1; \cdots; h_m) \), \( h_i : X \to \mathbb{R}, i = 1, \cdots, m \) are proper lower semicontinuous and convex functions, \( X \subseteq \mathbb{R}^n \) is a nonempty compact convex set. We call problem (1.1) either convex or nonconvex functional constrained optimization depending on whether \( f \) is convex or not. For the convex case, the objective function \( f \) is not necessarily differentiable. On the other hand, we assume \( f \) to be a differentiable function with Lipschitz continuous gradients for the nonconvex setting. The functional constrained problem in (1.1) can be used not only for the joint optimization of sparsity and risk aversion, but also for other penitential applications that require the trade-off of different requirements.

1.1. Motivation

We start with more detailed discussions about two motivating applications.

1. Portfolio Selection in Financial Engineering. As mentioned earlier, one notable example that is carried out with risk aversion and solution sparsity is portfolio selection with cardinality requirement. A set of risk efficient portfolios constructed from all available assets (see e.g., Markowitz 1959), however, raised the question of whether such an ideal policy is attainable. Indeed, due to various kinds of market friction such as transaction costs, taxes, regulations and asset indivisibility, common practice is to invest on a limited number of assets in a more realistic setting. To this end, cardinality requirement is imposed on the portfolio selection model with the goal to minimize the risk induced by a loss function \( \Psi(\cdot) \). One such formulation is give by

\[
\begin{align*}
    & \min \ \text{CVaR}[\Psi(x)] \\
    & \text{s.t. } \psi(x) \leq c, \\
    & x \in X,
\end{align*}
\]  

(1.2)

where \( \psi(\cdot) \) is a certain convex surrogate of cardinality constraint and \( c \) is the desired number of selected assets. Moreover, the problem in (1.2) can also be formulated as a nonconvex problem
with convex constraint, by replacing CVaR with VaR in the objective. Alternatively, the cardinality requirement can be modeled directly by the $\ell_0$-norm and participates in the objective function. To meet the cardinality constraint while minimizing the risk is a long-standing challenge in the area. Models and methodologies for cardinality constrained portfolio selection optimization have been developed in (Chang et al. 2000, Li et al. 2006, Bertsimas and Shioda 2009, Gao and Li 2013, Zheng et al. 2014). However, these integer programming oriented approaches are computationally inefficient when dealing with large-scale problems, although they may return exact solutions for smaller problems.

2. Intensity Modulated Radiation Therapy in Healthcare Analytics. Another important application of risk averse sparse optimization can be found in intensity modulated radiation therapy (IMRT) treatment plan in the area of healthcare analytics. This problem can be cast as a jointly sparse and risk averse optimization. In particular, the objective function of the optimization problem is formulated as a VaR, which represents a set of clinical criteria to avoid overdose (resp. underdose) to healthy (resp. tumor) tissues. In addition to a simplex constraint to induce a smaller number of apertures, it consists of a functional constraint, namely, a group sparsity constraint to enforce sparse angle/aperture selection in order to reduce the operation time and the radiation exposure to the patient (see e.g. Romeijn et al. (2005), Romeijn and Dempsey (2008), Lan et al. (2021) for more details of the problem description). Due to the huge dimensionality of the decision variable (e.g., the number of apertures), existing approaches suggest to approximate the risk averse requirement by some convex surrogate functions (e.g., quadratic penalty or CVaR). However, these methods barely return a solution that satisfies all clinical criteria, and often require a lot of fine-tuning of problem formulation (e.g., the penalty parameters). This motivates us to model the clinical criteria by employing a probabilistic form that constitutes the VaR measure as it is closer to the original clinical criteria (in terms of mathematical formula and interpretation) and to develop efficient algorithms to deal with the nonconvex model.

In spite of the importance of these models in applications, the algorithmic studies for solving these functional constrained problems are still limited. When the dimension of the decision variables $x$ is large, one natural choice for solving problem (1.1) would be first-order methods. These methods only require first-order information of the objective and constraint functions, and have been widely used in large-scale data analysis and machine learning applications due to their scalability. Most of these first-order methods require the projection over the feasible set $X$ (see Lan (2020)), which results in two significant limitations when applied to sparse optimization. First, the projection step often destroys the sparsity requirement in the sense that they cannot guarantee a sparse solution trajectory. Second, projection-based methods often require the computation of full gradients, which
can be computationally expensive, and sometimes is not even possible, as we will see in the IMRT problem.

To avoid these issues associated with projection-based algorithms, a common practice is to opt for the projection-free (a.k.a. conditional gradient) methods, which were pioneered in the work (Frank and Wolfe 1956) and subsequently developed in (Jaggi and Sulovský 2010, Harchaoui et al. 2012, Jaggi 2013, Lan 2013, Harchaoui et al. 2015, Freund and Grigas 2016). We refer to Lan et al. (2021) for a more comprehensive review of the method. Such algorithms eschew projections in favor of linear optimization. To be more specific, at each step, given the current iterate, these algorithms move towards an extreme point of a feasible set when optimizing a linear approximation of the objective function, and then update the iterate as a convex combination of the selected extreme points. As a consequence, each solution generated by these algorithms possesses sparse and low-rank properties. The generation of a sparse solution trajectory is one of the crucial properties that make projection-free methods stand out in sparse optimization. Another appealing property is that these algorithms only require the computation of one gradient component rather than the full gradient in many sparse optimization problems.

Unfortunately, the simplicity of existing projection-free methods comes with two major limitations. The first one is that it only demonstrates efficiency in convex problems with simple feasible set without functional constraints. To address this issue, Lan et al. (2021) proposed several novel constraint-extrapolated conditional gradient type methods (CoexCG and CoexDurCG) that handle the convex optimization with more involved functional constraints. However, these algorithms assume the existence of an optimal dual solution and the iteration complexity of the algorithms depends on the size of a possibly large optimal dual solution associated with the function constraints. The second significant limitation is the lack of efficient projection-free methods in dealing with nonconvex optimization problems with functional constraints.

1.2. Other Related Literature

1. Convex Functional Constrained Optimization. Methodologies developed for convex functional constrained problem lie in several lines. One research direction has been directed to exact/quadratic penalty and augmented Lagrangian methods (Bertsekas 1997, Lan and Monteiro 2013, 2016), etc., which require to solve the penalty subproblems and obtain the solutions therein. Instead of solving a more complicated penalty problem, a saddle-point reformulation of the original convex functional constrained problem is tackled by primal-dual type methods (Nemirovski 2004, Hamedani and Aybat 2021, Boob et al. 2022b). However, these methods require the projection over $X$ and depend on the dual space, whose diameter may be large. Alternatively, the convex problem
can be reformulated as a root finding problem and are suggested to be solved by level-set methods (Lemaréchal et al. 1995, Van Den Berg and Friedlander 2009, Van den Berg and Friedlander 2011, Aravkin et al. 2013, Harchaoui et al. 2015, Lin et al. 2018, Aravkin et al. 2019). In particular, Lin et al. (2018) developed a projection-based level-set method that maintains a feasible solution at each iteration. However, their method relies on a relatively strong assumption of feasibility guarantee and requires an estimate of the optimality gap of the problem. Other variants in solving the convex subproblems include accelerated gradient method (Nesterov 2018, Section 2.3.5) and bundle method (Lemarechal 1975, Wolfe 1975, Lan 2015), which resort to either an complicated quadratic program or a costly projection onto the feasible set.

2. Nonconvex Functional Constrained Optimization. Nonconvex problems have attracted much attention due to their empirical merits in important applications (see, e.g., Scutari et al. 2016, Boob et al. 2020). Algorithms are developed mainly in two different ways. One is to solve the problems indirectly within the framework of proximal point methods (Güler 1992, Bertsekas 2015, Lan and Yang 2019, Kong et al. 2019, Ma et al. 2019, Boob et al. 2022b), which approximate the problems with convex subproblems and may have nested structure that impedes efficient implementation. Direct approaches for solving nonconvex problems have also been studied in parallel (see e.g., Ghadimi and Lan (2013, 2016), Allen-Zhu and Hazan (2016), Reddi et al. (2016), Carmon et al. (2018)). However, these methods mainly focus on solving unconstrained problems or problems with simple feasible sets, which are not applicable to our setting. Existing methods for nonconvex optimization with function constraints all require projections (see, e.g., Boob et al. (2022a) and references therein), whereas current projection-free methods can only handle simple feasible sets for nonconvex optimization (see, e.g., Jiang et al. (2019) and (Lan 2020, Section 7.1)).

1.3. Contributions and Outline

Our contributions in this paper are briefly summarized as follows.

Firstly, we propose a novel projection-free method, referred to as Level Conditional Gradient (LCG) method, for solving convex functional constrained optimization. Different from the constraint-extrapolated conditional gradient type methods (CoexCG and CoexDurCG) developed in (Lan et al. 2021), LCG, as a primal method, does not assume the existence of an optimal dual solution, thus improving the convergence rate of CoexCG/CoexDurCG by eliminating the dependence on the size of the optimal dual solution. Similar to existing level-set methods, LCG uses an approximate Newton method to solve a root-finding problem. In each approximate Newton update, LCG calls a conditional gradient oracle (CGO) to solve a saddle point subproblem. The CGO developed herein employs easily commutable lower and upper bounds on these saddle point problems. We establish the iteration complexity of the CGO for solving a general class of saddle
point optimization. Using these results, we show that the overall iteration complexity of the proposed LCG method is bounded by $O\left(\frac{1}{\varepsilon^2} \log\left(\frac{1}{\varepsilon}\right)\right)$ for finding an $\varepsilon$-optimal and $\varepsilon$-feasible solution of problem (1.1). To the best of our knowledge, LCG is the first primal conditional gradient method for solving convex functional constrained optimization. For the subsequently developed nonconvex algorithms in this paper, LCG can also serve as a subroutine or provide high-quality starting points that expedites the solution process.

Secondly, to cope with the nonconvex functional constrained optimization problems (when $f$ is nonconvex in (1.1)), we develop two approaches: the Level Inexact Proximal Point (IPP-LCG) method and the Direct Nonconvex Conditional Gradient (DNCG) method. The proposed IPP-LCG method utilizes the proximal point framework and solve a series of convex subproblems. By solving each subproblem, it leverages the proposed LCG method, thus possessing the preponderance in averting the effect from large Lagrangian multipliers. We show that the iteration complexity of the algorithm is bounded $O\left(\frac{1}{\varepsilon^3} \log\left(\frac{1}{\varepsilon}\right)\right)$ in order to obtain an $(\varepsilon,\varepsilon)$-KKT point. However, the proximal-point type method has triple-layer structure and may not be easily implementable. To alleviate the issue, we also propose the DNCG method, which is the first single-loop projection-free algorithm for solving nonconvex functional constrained problem in the literature. This algorithm provides a drastically simpler framework as it only contains three updates in one loop. We show that the iteration complexity to find an $\varepsilon$-Wolfe point is bounded by $O(1/\varepsilon^4)$. To the best of our knowledge, all these developments are new for projection-free methods for nonconvex optimization.

Finally, we present novel convex and nonconvex functional constrained models that are well-suited to risk averse sparse optimization problems in portfolio selection and IMRT treatment planning. These models incorporate different types of risk aversion and sparsity requirements and can be solved efficiently by our proposed algorithms. For the portfolio selection problem with cardinality requirement, our numerical experiments show that all algorithms (LCG, IPP-LCG, DNCG) are efficient in jointly minimizing the risk while lowering cardinality of the selected assets in a rather short computational time for real-world and large-scale datasets. For the IMRT application, the proposed DNCG method, equipped with initial points output from LCG, satisfies the requirement of meeting a set of very challenging clinical criteria and selecting sparse angles in order to reduce the radiation time, which accounts for a reasonable treatment plan. It is worth mentioning that such requirements could not be satisfied by using any existing methods developed in the literature (e.g., (Romeijn et al. 2005, Romeijn and Dempsey 2008, Lan et al. 2021)).

The rest of the paper is organized as follow. In Section 2, we introduce the Level Conditional Gradient method targeting for solving a class of convex constrained problems. Next in Section 3, for a class of nonconvex problems, we present the Level Inexact Proximal Point method and the Direct Nonconvex Conditional Gradient method. We then apply these methods to the portfolio
The following notations will be used throughout the paper.

- Without specific mention, \(\|\cdot\|\) denotes arbitrary norm (not necessarily associated with the inner product) in the Euclidean space and \(\|\cdot\|_1\), denotes its conjugate.
- For a closed convex set \(X \subset \mathbb{R}^n\), the set \(N_X(x)\) denotes the normal cone at \(x \in X\) and \(N_X(x) := \{g \in \mathbb{R}^n | \forall z \in X : g^T(z - x) \leq 0\}\).
- A function \(f : \mathbb{R}^n \to \mathbb{R}\) is \(L_f\)-smooth if \(\|\nabla f(x_1) - \nabla f(x_2)\|_2 \leq L_f \|x_1 - x_2\|, \forall x_1, x_2 \in X\).
- A function \(f : \mathbb{R}^n \to \mathbb{R}\) is \(M_f\)-Lipschitz continuous if \(|f(x_1) - f(x_2)| \leq M_f \|x_1 - x_2\|, \forall x_1, x_2 \in X\).
- Suppose \(x^*\) is an optimal solution of (1.1). \(\bar{x}\) is an \(\epsilon\)-optimal and \(\epsilon\)-feasible solution (or \(\epsilon\)-solution) of (1.1) if \(\bar{x} \in X, f(\bar{x}) - f(x^*) \leq \epsilon\) and \(\|h(\bar{x})\|_\infty \leq \epsilon\).

2. Convex Conditional Gradient Method

In this section, we introduce the Level Conditional Gradient (LCG) method that solves the convex constrained optimization problem (1.1) and establish its convergence rate.

It is well-known that problem (1.1) can be reduced to a root finding problem. For a given level estimate \(l \in \mathbb{R}\), let us define

\[
\phi(l) := \min_{x \in X} \max \{f(x) - l, h_1(x), \ldots, h_m(x)\} \\
= \min_{x \in X} \gamma \max_{(\gamma, z) \in Z} \gamma [f(x) - l] + \sum_{i=1}^m z_i h_i(x). \tag{2.1}
\]

Here \(Z := \{(\gamma, z) \in \mathbb{R}^{m+1} : \gamma + \sum_{i=1}^m z_i = 1, \gamma, z_i \geq 0\}\) denotes the standard simplex. We can easily verify that: (a) \(\phi(l)\) is monotonically non-increasing and convex w.r.t. \(l\); (b) \(\phi(f^*) = 0\); (c) \(\phi(l) \geq 0\) for any \(l \leq f^*\) and \(\phi(l) \leq 0\) for any \(l \geq f^*\). Therefore, problem (1.1) is equivalent to finding the root of \(\phi(l) = 0\).

We propose to solve (1.1) by LCG (see Algorithm 1), which consists of an outer loop that updates the level estimate \(l\) (i.e., the estimation of \(f^*\)), and an inner loop that calls a specialized conditional gradient oracle (CGO) to solve the saddle point problem in (2.1) given a level estimate \(l\).

2.1. Outer Loop of LCG

The basic idea of the LCG method is to apply an approximate Newton’s method to solve \(\phi(l) = 0\). Assume for the moment that problem (2.1) can be solved exactly for any given \(l_k\). Then one can compute the function value \(\phi(l_k)\), a subgradient \(\phi'(l_k)\). Solving the following linear equation

\[
\phi(l_k) + \phi'(l_k)(l - l_k) = 0
\]
gives us an updated iterate $l_{k+1}$ as

$$l_{k+1} = l_k - \frac{\phi(l_k)}{\phi'(l_k)}.$$

Since $\phi(l)$ cannot be computed exactly, we suggest to use a computable lower bound and an approximate subgradient in place of $\phi(l_k)$ and $\phi'(l_k)$ in the above equation, respectively. Started with an initial level estimate $l_1 \leq f^*$, we call CGO to compute a lower bound $L_k$, an upper bound $U_k$ of $\phi(l_k)$ and an approximate pair of solutions $(x_k; (\gamma_k, z_k)) \in X \times Z$ of problem (2.1) at the $k$-th iteration (see Algorithm 1). A gap defined by these bounds (i.e. $U_k - L_k$) indicates how accurately problem (2.1) (with $l = l_k$) is solved. Whenever the upper bound $U_k \leq \epsilon$, LCG terminates since an approximate root of $\phi(l) = 0$ has been found due to $\phi(l_k) \leq U_k \leq \epsilon$ and $\phi(l_k) \geq 0$. Otherwise, the algorithm updates the level estimate $l_k$. More specifically, we define the following linear function as a lower approximation of $\phi(l)$, $\forall l \in \mathbb{R}$:

$$L_k(l) := L_k - \gamma_k (l - l_k). \quad (2.2)$$

Intuitively, $L_k(l)$ underestimates $\phi(l)$ since $-\gamma_k$ and $L_k$ respectively serve as an approximate subgradient and a lower bound for $\phi(\cdot)$ at $l = l_k$. To perform the approximate Newton’s step as mentioned earlier, we solve $L_k(l) = 0$ and obtain the following update of the level estimate

$$l_{k+1} = l_k + \frac{1}{\gamma_k}L_k. \quad (2.3)$$

We note that the LCG method provides a general framework for solving the root finding problem in (2.1) and is not restricted to a particular inner oracle, as long as the output $(\gamma_k, L_k, U_k)$ of the inner oracle (e.g., CGO) satisfies the following conditions:

$$\gamma_k > 0, \quad (2.4)$$

$$L_k \leq \phi(l_k) \leq U_k, \quad (2.5)$$

$$L_k(l) \leq \phi(l), \forall l. \quad (2.6)$$

The following lemma states an important property of the sequence of the level estimates $(l_k)_{k \geq 1}$ generated in the outer loop of the algorithm. Such property will be used in establishing the number of outer loops required by the LCG method.

**Lemma 2.1.** At iteration $k$, if Algorithm 1 does not terminate, then $L_k > 0$. Moreover, the sequence of the level estimates satisfies $l_1 < \cdots < l_k < l_{k+1} < \cdots \leq f^*$, $k \geq 1$. Consequently, $\phi(l_{k+1}) \geq \phi(l_k) \geq \cdots \geq \phi(f^*) = 0$. 
Algorithm 1 Level Conditional Gradient Method (LCG)

1: Inputs: $\epsilon > 0, \mu \in (\frac{1}{2}, 1)$.
2: Initialization: $x_0 \in X, l_1 = \{ \min f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle : x \in X \}$.
3: for $k = 1, 2, \ldots$ do
4: Call CGO with input $l_k$ and obtain approximate solutions $(x_k; (\gamma_k, z_k)) \in X \times Z$, lower bound $L_k$, upper bound $U_k$ such that $U_k - L_k \leq (1 - \mu)\epsilon$.
5: if $U_k \leq \epsilon$ then
6: Terminate and return $x_k$.
7: end if
8: $l_{k+1} = l_k + \frac{1}{\gamma_k}L_k$.
9: end for

Remark 2.1. In LCG, we require that the initial level estimate satisfies $l_1 \leq f^\star$. Otherwise, the algorithm terminates at the first outer iteration. To see this, if $l_1 \geq f^\star$, then $L_1 \leq \phi(l_1) \leq \phi(f^\star) = 0$, which holds because $L_1$ is the lower bound of $\phi(l_1)$ and $\phi$ is a non-increasing function. Hence by the stopping criteria of CGO, $U_1 \leq L_1 + (1 - \mu)\epsilon \leq \epsilon$, which results in the termination of the algorithm. It should be noted that, by slightly modifying the outer scheme of LCG, it is also possible to approximate $f^\star$ from above starting with an initial level $l_1 \geq f^\star$. More details are provided in Appendix A.3.

In the theorem below, we establish the iteration complexity of reaching “$U_k \leq \epsilon$”, which is essentially the outer loop iteration complexity of solving (1.1) by Algorithm 1.

Theorem 2.1. For all $k \geq 1$, we have

$$U_k \leq (f^\star - l_1) \frac{1}{2\mu} \left( \frac{1}{1 - 2\mu} \right)^k,$$

where $\mu \in (\frac{1}{2}, 1), l_1$ is the initial estimate of the optimal value of (1.1) such that $l_1 \leq f^\star$. Moreover, given precision $\epsilon$, at the termination of LCG when $U_k \leq \epsilon$, the algorithm yields an $\epsilon$-optimal and $\epsilon$-feasible solution $x_k$ of problem (1.1).

2.2. Conditional Gradient Oracle for Smooth Functions

In this section, we introduce the Conditional Gradient Oracle (CGO) for solving the following saddle point problem

$$\bar{\phi} := \min_{x \in \bar{X}} \max_{z \in \bar{Z}} \bar{f}(x) + \langle \bar{h}(x), z \rangle.$$

where $\bar{f}, \bar{h} : \bar{X} \to \mathbb{R}$ and $\bar{h} : \bar{X} \to \mathbb{R}^\bar{m}$ are proper lower semicontinuous convex functions, $\bar{X} \subseteq \mathbb{R}^\bar{n}$ is a nonempty compact convex set, and $\bar{Z} \subseteq \mathbb{R}^\bar{m}$ is a general compact set. Under these assumptions an
optimal pair of solutions \((x^*, z^*) \in \bar{X} \times \bar{Z}\) of problem (2.8) must exist. Clearly, the subproblem in (2.1) can be viewed as a special case of problem (2.8) with \(\bar{f} = 0, \bar{X} = X, \bar{Z} = Z\) and \(\bar{h} = (f - l, h)\).

We assume in this subsection that \(\bar{f}\) is an \(L_{\bar{f}}\)-smooth, \(M_{\bar{f}}\)-Lipschitz continuous function and \(\bar{h}_i\) is an \(L_{\bar{h}_i}\)-smooth, \(M_{\bar{h}_i}\)-Lipschitz continuous function, \(i = 1, \ldots, m\). It should be noted that CGO can also be extended to nonsmooth problems with certain structure. More details of the nonsmooth setting are provided in Appendix A.1.3.

Let \(\nu : \bar{Z} \to \mathbb{R}\) be a 1-strongly convex and \(L_{\nu}\)-smooth distance generating function and define the proximal function at point \(z' \in \bar{Z}\) as

\[
\nu(z) = \nu(z) - \langle \nabla \nu(z'), z - z' \rangle, \quad z, z' \in \bar{Z}.
\]

Further, denote the linear approximation of \(\bar{f}\) and \(\bar{h}_i\) at \(x'\) as

\[
\ell_{\bar{f}}(x', x) := \bar{f}(x') + \langle \nabla \bar{f}(x'), x - x' \rangle,
\]

\[
\ell_{\bar{h}_i}(x', x) := \bar{h}_i(x') + \langle \nabla \bar{h}_i(x'), x - x' \rangle, \quad i = 1, \ldots, m.
\]

The algorithmic scheme of CGO is stated in Algorithm 2. Through step (2.9) - (2.13), it first extrapolates the linear approximation of the convex functions \(\bar{h}\) controlled by the weight \(\lambda_t\), then updates the dual variable \(r_t\) based on the extrapolated value \(\tilde{h}_t\) and the proximal function \(V\). En route, CGO computes the primal variable \(p_t\) by minimizing the a linear function over \(\bar{X}\) and determines the solution \(x_t\) by taking the convex combination of \(p_t\) and \(x_{t-1}\). Then it recursively computes the lower bounding functions \(f_t(\cdot)\) and \(h_t(\cdot)\) of \(\bar{f}(\cdot)\) and \(\bar{h}(\cdot)\), respectively in (2.14) and (2.15), with \(\underline{f}_t(\cdot)\) and \(\underline{h}_t(\cdot)\) respectively initialized as lower linear approximation of \(\bar{f}(\cdot)\) and \(\bar{h}(\cdot)\) at the initial point (see Lemma 2.2 for a formal proof). Finally in (2.16) and (2.17), CGO generates a lower bound \(L_t\) and an upper bound \(U_t\) of (2.8) by solving simple linear programs.

It is worth mentioning the relationship between CGO and the CoexCG/CoexDurCG algorithm in (Lan et al. 2021). Both CoexCG and CGO share a similar routine of updating the primal and dual variables from the perspective of applying projection-free technique. The main differences of these two algorithms lie in the following several fronts. First, CGO computes the lower and upper bounds of the saddle point problem and terminates when these two bounds are close enough. CGO neither requires the knowledge of the total number of iterations as it is the case for CoexCG, nor does it need to perform additional regularization in the dual update, as it is the case for CoexDurCG. Second, CoexCG is designed to solve the functional constrained problem while CGO aims for the saddle point problem. In the special case of solving the subproblem (2.1), the dual space \(Z\) that CGO operates on is a simplex so that its convergence rate is not affected by large Lagrangian multipliers, as opposed to CoexCG. Third, as an inner oracle in solving the convex constrained problem, CGO outputs the dual solution \(z_t\), which participates in the update of level estimate \(l\) in the outer loop. In CoexCG, the dual variable is created merely as a tool for the convergence analysis.
Algorithm 2 Conditional Gradient Oracle (CGO)

Parameters: \( \lambda_t \geq 0, \tau_t \geq 0, \alpha_t \in [0, 1], \alpha_1 = 1, \epsilon > 0, \mu \in (\frac{1}{2}, 1) \).

Initialization: \( x_{-2} = x_{-1} = x_0 \in \bar{X}, p_{-1} = p_0 \in \bar{X}, z_0 = r_0 = \bar{Z}, f_p(x) \leq \bar{f}(x), h_0(x) \leq \bar{h}(x) \).

for \( t = 1, 2, \ldots \) do

Compute \( z_t, x_t, L_t \) and \( U_t \) according to

\[
\bar{h}_t = \ell_h(x_{t-2}, p_{t-1}) + \lambda_t[\ell_h(x_{t-1}, p_{t-1}) - \ell_h(x_{t-3}, p_{t-2})],
\]

(2.9)

\[
r_t = \arg\min_{z \in \bar{Z}} (\bar{h}_t, z) + \tau V(r_{t-1}, z),
\]

(2.10)

\[
z_t = (1 - \alpha_t)z_{t-1} + \alpha_tr_t,
\]

(2.11)

\[
p_t = \arg\min_{x \in \bar{X}} \ell_f(x_{t-1}, x) + \langle \ell_h(x_{t-1}, x), r_t \rangle,
\]

(2.12)

\[
x_t = (1 - \alpha_t)x_{t-1} + \alpha_tp_t,
\]

(2.13)

\[
f_p(x) = (1 - \alpha_t)f_{p-1}(x) + \alpha_t\ell_f(x_{t-1}, x),
\]

(2.14)

\[
h_p(x) = (1 - \alpha_t)h_{p-1}(x) + \alpha_t(\ell_h(x_{t-1}, x), r_t),
\]

(2.15)

\[
L_t = \min_{x \in \bar{X}} f_p(x) + h_{p}(x),
\]

(2.16)

\[
U_t = \max_{z \in \bar{Z}} \bar{f}(x_t) + \langle \bar{h}(x_t), z \rangle.
\]

(2.17)

if \( U_t - L_t \leq (1 - \mu)\epsilon \) then

Terminate and return \( x_t, z_t, L_t, U_t \).

end if

end for

In the remaining part of this subsection, we discuss the convergence properties of CGO.

The following lemma shows that \( L_t \) and \( U_t \), \( t = 1, 2, \ldots \), are valid lower bounds and upper bounds of (2.8), respectively.

**Lemma 2.2.** Let \( \bar{\phi} \), \( L_t \) and \( U_t \) be defined in (2.8), (2.16) and (2.17), respectively. Also let \( z_t \) be defined in (2.11). Then we have

\[
f_p(x) \leq \bar{f}(x),
\]

(2.18)

\[
h_p(x) \leq \langle \bar{h}(x), z_t \rangle,
\]

(2.19)

\[
L_t \leq \bar{\phi} \leq U_t,
\]

(2.20)

for any \( t \geq 1 \).

In view of Lemma 2.2, \( (f_p + h_p)(\cdot) \) provides a lower bound for the objective of (2.8), i.e., \( (f_p + h_p)(\cdot) \leq \bar{f}(x_t) + \langle \bar{h}(x_t), z \rangle \). This motivates us to define the gap function for problem (2.8) as

\[
\bar{Q}_t(w, w) := \bar{f}(x_t) + \langle \bar{h}(x_t), z \rangle - f_p(x) - h_p(x),
\]

(2.21)
where \( w_t := (x_t, z_t) \), \( w := (x, z) \). Also, by the definition of \( L_t \) and \( U_t \), we can easily see that
\[
\max_{w \in \bar{X} \times \bar{Z}} \hat{Q}_t(w_t, w) = U_t - L_t.
\]
It is worth mentioning here that the gap function in (2.21) is different from those used in the existing literature, given by
\[
\hat{Q}_t(w_t, w) := \bar{f}(x_t) + \langle \bar{h}(x_t), z \rangle - \bar{f}(x) - \langle \bar{h}(x), z_t \rangle.
\]
As a consequence, these algorithms require the solution of \( \min_{x \in \bar{X}} (\bar{f}(x) + \langle \bar{h}(x), z_t \rangle) \) to compute a lower bound on \( \phi \), which can be computationally expensive unless both \( \bar{f} \) and \( \bar{h} \) are simple enough (e.g., linear functions). On the other hand, the computation of the lower bound \( L_t \) in CGO only requires one call to the linear optimization oracle. In addition, since \( \bar{Q}_t(w_t, w) \geq \tilde{Q}_t(w_t, w) \), we obtain stronger convergence guarantees for the developed algorithm by using \( \bar{Q}_t(w_t, w) \) instead of \( \tilde{Q}_t(w_t, w) \) as the error measure.

Theorem 2.2 below states the main convergence properties for CGO. For simplicity, we focus on the setting where \( \bar{f} \) and \( \bar{h} \) are smooth convex functions (see Appendix A.1.3 for the discussion on the nonsmooth setting). We need to use the following quantities for this result:
\[
\bar{M} := \left( \sum_{i=1}^{m} M_{h_i}^2 \right)^{1/2}, \quad D_{\bar{X}} := \max_{x_1, x_2 \in \bar{X}} \|x_1 - x_2\| \quad \text{and} \quad \nabla := \max_{z_1, z_2 \in \bar{Z}} V(z_1, z_2).
\]

**THEOREM 2.2.** Suppose that the algorithmic parameters in CGO are set to
\[
\alpha_t = \frac{2}{t + 1}, \quad \lambda_t = \frac{t - 1}{t}, \quad \tau_t = 9\sqrt{t}MD_{\bar{X}}, \quad t \geq 1.
\]

Then for any \( t \geq 1 \),
\[
\bar{Q}_t(w_t, w) \leq \frac{2(L_{\bar{f}} + z^T L_{\bar{h}})D_{\bar{X}}^2}{t + 1} + \frac{MD_{\bar{X}}}{\sqrt{t + 1}} \left[ 18\nabla + \frac{7}{6} \right] \forall w \in (\bar{X}, \bar{Z}).
\]

### 2.3. Overall Complexity

In this section, we present the overall iteration complexity of the LCG method applied to the convex functional constrained problem in (1.1) with subproblem (2.1) solved by CGO.

As mentioned in Section 2.2, when we apply CGO for solving subproblem (2.1), we have \( \bar{f}(x) = 0 \), \( \bar{h}(x) \equiv \bar{h}(x; l) = (f(x) - l, h(x)) \) for a given level estimate \( l \), \( \bar{X} = X \) and \( \bar{Z} = Z \). In the following lemma we show that the output of CGO satisfies the conditions (2.4)-(2.6) to guarantee the convergence of the outer loop of LCG.
Lemma 2.3. When LCG does not terminate at iteration \( k \), the output \((\gamma_k, L_k, U_k)\) of CGO satisfies (2.4)-(2.6).

We are now ready to establish the overall iteration complexity of the LCG method.

Theorem 2.3. Suppose that the algorithmic parameters of CGO are set to (2.22). Then the total number of CGO iterations required to find an \( \epsilon \)-solution \( \bar{x} \in X \) of (1.1) can be bounded by \( O \left( \frac{1}{\epsilon^2} \log \left( \frac{1}{\epsilon} \right) \right) \).

Remark 2.2. It is worth mentioning here that as the output solution \( x_k \) may not be a feasible solution such that \( h(x_k) \leq 0 \), we develop a lower bound for \( f(x_k) - f^* \), which is presented in Lemma A.1.4 in Appendix A.1.1.

3. Nonconvex Conditional Gradient Methods

In this section, we focus on the nonconvex functional constrained problem (1.1), where \( f \) is nonconvex and \( h_i, i = 1, \cdots, m \) are convex. Due to the difficulty of solving the nonconvex functional constrained optimization to global optimality (even to local optimality), we seek an approximate stationary points of problem (1.1). We introduce two methods to solve this problem: Inexact Proximal Point Level Conditional Gradient (IPP-LCG) and Direct Nonconvex Conditional Gradient (DNCG).

Throughout the section, we make the following assumptions: (a) \( f \) is \( L_f \)-smooth and \( M_f \)-Lipschitz continuous; (b) \( h_i \) is \( L_{h_i} \)-smooth and \( M_{h_i} \)-Lipschitz continuous; (c) \( f \) satisfies a lower curvature condition such that

\[
f(x) - f(y) - \langle \nabla f(y), x - y \rangle \geq -\frac{L_f}{2} \|x - y\|^2, \forall x, y \in X.
\] (3.1)

Here we assume that \( \|\cdot\| \) is an inner product norm in this section for the sake of simplicity.

3.1. Inexact Proximal Point Method

The main idea of the IPP-LCG method is to leverage the LCG method (see Section 2) to inexactely solve a sequence of convex subproblems that approximate the original nonconvex problem. More specifically, given the current iterate \( x_{j-1} \in X \), we solve the following convex subproblem:

\[
\begin{align*}
\min_{x'} & \quad f(x; x') := f(x) + L_f \|x - x_{j-1}\|^2 \\
\text{s.t.} & \quad h_i(x) \leq 0, \quad i = 1, \cdots, m, \\
& \quad x \in X.
\end{align*}
\] (3.2)

We assume that the Slater conditions holds for (3.2), i.e., \( \exists \tilde{x} \in X \) such that \( h_i(\tilde{x}) < 0, \quad i = 1, \cdots, m \), and use \((x_j^*, y_j^*)\) to denote a pair of its primal and dual solutions. As described in Algorithm
3, at the \( j \)-the iteration the IPP-LCG method calls LCG to solve subproblem (3.2) to obtain a \((\delta^f, \delta^h)\)-optimal solution \( x_j \) s.t.

\[
f(x_j; x_{j-1}) - f(x_j^*; x_{j-1}) \leq \delta^f; \| [h(x_j)]_+ \| \leq \delta^h.
\]

Among all the candidate solutions across iterations, the method picks \( \hat{x}_j \) such that \( \hat{j} \in \arg\min_{j=1,\ldots,J} f(x_{j-1}) - f(x_j) \) as the output solution.

**Algorithm 3** Inexact Proximal Point Level Conditional Gradient Method (IPP-LCG)

Initialization: \( x_0 \in X \).

for \( j = 1, 2, \ldots, J \)

Call LCG to solve (3.2) and return a \((\delta^f, \delta^h)\)-optimal solution \( x_j \).

end for

Select \( \hat{j} \) such that \( \hat{j} \in \arg\min_{j=1,\ldots,J} f(x_{j-1}) - f(x_j) \).

Terminate and return \( x_{\hat{j}} \).

We use the following criterion to measure the progress of the IPP-LCG method.

**Definition 3.1.** For problem (1.1),

(i) \( x' \) is an \((\epsilon, \delta)\)-KKT point if \( x' \in X \) and there exists \((x, y)\) such that \( h_i(x) \leq 0, x \in X, y_i \geq 0, i = 1, \cdots, m \) and

\[
\sum_{i=1}^{m} |y_i h_i(x)| \leq \epsilon,
\]

\[
\left[ d \left( \nabla f(x) + \sum_{i=1}^{m} y_i \nabla h_i(x), - N_X(x) \right) \right]^2 \leq \epsilon,
\]

\[
\| x' - x \|^2 \leq \delta,
\]

where \( \epsilon, \delta > 0, d(\cdot, \cdot) \) denotes the distance between two sets \( A \) and \( B \) such that \( d(A, B) := \min_{a \in A, b \in B} \| a - b \| \); 

(ii) \( x \) is an \( \epsilon \)-KKT point (paired with \( y \)) if it satisfies the first two criteria in (3.3) with \( h_i(x) \leq 0, x \in X, y_i \geq 0, i = 1, \cdots, m \).

We are now ready to present the convergence result for the IPP-LCG method.

**Theorem 3.1.** The total number of CGO iterations performed by the IPP-LCG method to compute an \((\epsilon, \epsilon)\)-KKT point of problem (1.1) is bounded by \( O \left( \frac{1}{\epsilon^3 \log(\frac{1}{\epsilon})} \right) \).

Note that given a target accuracy \( \epsilon > 0, \delta^f \) and \( \delta^h \) can be selected as in the order of \( \epsilon \) such that \( \delta^f = O(\epsilon) \) and \( \delta^h = O(\epsilon) \). Moreover, the iteration number \( J \) can be fixed to \( O(1/\epsilon) \).
It is worth noting that IPP-LCG can also be generalized to solve structured nonsmooth problems by applying LCG on the nonsmooth convex subproblems. The convergence analysis in this case is more or less the same as that shown in Theorem 3.1.

Observe that IPP-LCG is a triple-layer algorithm as we add an extra proximal point approximation loop on top of LCG, which already contains one inner oracle and an outer loop. Hence, it is not very convenient to implement this algorithm. In the next subsection, we present a more concise and easily implementable algorithm to solve problem (1.1) in the nonconvex setting.

3.2. Direct Nonconvex Conditional Gradient Method

To tackle the nonconvex functional constrained optimization (1.1), one alternative is to solve its Lagrangian dual given by

\[
\min_{x \in X} \max_{y \in \mathbb{R}^m_+} \{ F(x, y) := f(x) + \sum_{i=1}^{m} y_i h_i(x) \}. \tag{3.4}
\]

In general, \( F \) in (3.4) is nonsmooth in \( x \) and can be approximated by a smooth function

\[
\tilde{F}(x) := f(x) + \sum_{i=1}^{m} y_i(x) h_i(x) - \frac{c}{2} \|y(x)\|^2, \quad \text{with } y(x) := \arg\max_{y(x) \in \mathbb{R}^m_+} \tilde{F}(x) \tag{3.5}
\]

as shown in Lemma 3.1 below.

**Lemma 3.1.** \( \tilde{F}(\cdot) \) is a smooth function such that \( \|\nabla \tilde{F}(x_1) - \nabla \tilde{F}(x_2)\| \leq L_c \|x_1 - x_2\|, \forall x_1, x_2 \in X, \)

where \( L_c := L_f + \frac{\|M_h\|_c \|L_h\|_{P_X}}{c} + \frac{\|M_h\|^2}{c}, \ L_h := (L_{h_1}, \cdots, L_{h_m}), \ M_h := (M_{h_1}, \cdots, M_{h_m}) \) and \( c > 0. \)

Note that, given \( x \), we can obtain the closed form solution of \( y(x) \) in (3.5) such that \( y(x) = \max \left\{ \frac{h(x)}{c}, 0 \right\}. \) The DNCG method (detailed in Algorithm 4) directly applies the conditional gradient method on the following approximation problem:

\[
\min_{x \in X} \tilde{F}(x). \tag{3.6}
\]

More specifically, DNCG takes \( x_0 \) as input and calculates \( y_0 \) using the closed form. Then in each iteration it computes the primal solution \( x_k \) by calling the linear optimization oracle in (3.7) and performing convex combination in (3.8). Finally it updates the dual solution \( y_k \) in (3.9).

To evaluate the efficiency of the DNCG method applied on problem (1.1) at \( \bar{x} \in X \), we use the following error measures:

**Definition 3.2.** Given a target accuracy \( \epsilon > 0, \) \( \bar{x} \in X \) is an \( \epsilon \)-Wolfe point if

\[
Q(\bar{x}) := \max_{x \in X} \langle \nabla \tilde{F}(\bar{x}), \bar{x} - x \rangle \leq \epsilon, \\
\| h(\bar{x}) \|_+^2 \leq \epsilon. \tag{3.10}
\]
Algorithm 4 Direct Nonconvex Conditional Gradient Method (DNCG)

Inputs: $c > 0$.
Initialization: $x_0 \in X$, $y_0 = \max \left\{ \frac{h(x_0)}{c}, 0 \right\}$.

for $k = 1, 2, \ldots, K$ do

\[ p_k = \arg\min_{x \in X} \langle \nabla F(x_{k-1}), x - x_{k-1} \rangle, \quad (3.7) \]

\[ x_k = (1 - \alpha_k)x_{k-1} + \alpha_k p_k, \quad (3.8) \]

\[ y_k = \max \left\{ \frac{h(x_k)}{c}, 0 \right\}. \quad (3.9) \]

end for

The function $Q(\bar{x})$ in (3.10), often referred to as the Wolfe gap in projection-free methods, corresponds to the first-order optimality condition of problem (3.6). This explains why we call $\bar{x} \in X$ satisfying (3.10) an $\epsilon$-Wolfe point. By the definition of $\bar{F}$, we have $\nabla \bar{F}(\bar{x}) = \nabla f(\bar{x}) + \sum_{i=1}^{m} y_i(\bar{x}) \nabla h_i(\bar{x})$. Hence this first criterion in (3.10) also tells us how the stationarity of the KKT condition of problem (1.1) is satisfied for a given pair of primal and dual solution $(\bar{x}, y(\bar{x})) \in X \times \mathbb{R}^m$. The second criteria characterizes the constraint violation at $\bar{x}$. Note that the $\epsilon$-Wolfe point defined above provides no guarantee of complementary slackness for the KKT condition of (1.1).

It is worth pointing out here the relationship between the convergence criteria used by DNCG (see (3.10)) and the one by IPP-LCG (see (3.3)). If $x'$ is an $\epsilon$-KKT point (see Definition 3.1 (ii)), then $h(x') \leq 0$, so that $\|[h(x')]_+\|^2 \leq 0$, which implies the second condition of the $\epsilon$-Wolfe point. For some $y \geq 0$, let $r = \nabla f(x') + \sum_{i=1}^{m} y_i \nabla h_i(x')$. Since $[d(r, -N_X(x'))]^2 \leq \epsilon$, then we can find some $g \in -N_X(x')$ such that $\|g - r\|^2 = \epsilon$ and $\langle g, x - x' \rangle \geq 0, \forall x \in X$. Consequently, $\forall x \in X,$

\[ \langle g - r, x' - x \rangle + \langle r, x' - x \rangle \leq 0. \quad (3.11) \]

Let $z' \in \arg\max_{x \in X} \langle r, x' - x \rangle.$ From (3.11), we have

\[ \max_{x \in X} \langle r, x' - x \rangle \leq \langle g - r, z' - x' \rangle. \quad (3.12) \]

Square both sides in (3.12), we obtain

\[ \left( \max_{x \in X} \langle r, x' - x \rangle \right)^2 \leq \|g - r\|^2 \|z' - x'\|^2 \leq \epsilon D_X^2. \quad (3.13) \]

The result in (3.13) implies that $(Q(x'))^2 \leq \epsilon D_X^2$, and thus $Q(x') \leq \sqrt{\epsilon} D_X.$

Note that an $\epsilon$-KKT point inherits complimentary slackness, which is not a condition for an $\epsilon$-constrained Wolfe point. However, such $\epsilon$-KKT point is not explicitly computed by IPP-LCG and
it is only used to be measured against the output solution under some distance, while an \( \epsilon \)-Wolfe point directly associates with the computed solution of DNCG.

We are now ready to analyze the convergence rate of the DNCG algorithm based on the criteria in (3.10).

**Theorem 3.2.** The total number of iterations required to compute an approximate solution \( \bar{x} \) such that \( Q(\bar{x}) \leq \epsilon \) and \( \| [h(\bar{x})]_+ \| \leq \epsilon \) is bounded by \( O(1/\epsilon^4) \).

We can also generalize DNCG to solve problems with nonsmooth \( h(\cdot) \) by using the Nesterov smoothing scheme (see more details in Appendix A.4.2).

## 4. Numerical Experiments

In this section, we demonstrate the efficiency of the proposed algorithms (LCG, IPP-LCG and DNCG) in two important applications: portfolio selection and the intensity modulated radiation therapy (IMRT) treatment planning. Numerical comparison with CoexDurCG are also provided. All experiments are run using Python 3.8.5 under the Ubuntu 20.04.1 LTS operating system with a 4.20 GHz Intel Core i7 processor and 32Gb RAM.

### 4.1. Portfolio Selection

In this section, we first introduce the portfolio selection problem with and without cardinality constraint, and then apply LCG, IPP-LCG and DNCG to solve the formulated convex and nonconvex models using the real-world stock market dataset.

**4.1.1. Models** Consider selecting portfolio among \( N \) risky assets with random return \( r_i, i = 1, \cdots, N \) and random target return \( R \) (a.k.a. market index). Let \( x_i \) be the decision variable that determines the weight of the \( i \)-th asset to be chosen, \( i = 1, \cdots, N \), such that \( \sum_{i=1}^{N} x_i \leq 1 \). The goal is to minimize the risk that the overall return is below the target return in expectation, i.e., \( \mathbb{E} \left[ \mathbb{1}\{ R - \sum_{i=1}^{N} r_i x_i > 0 \} \right] \), or, equivalently, \( P \left( R - \sum_{i=1}^{N} r_i x_i > 0 \right) \), where \( \mathbb{1}\{ x > 0 \} = 1 \) if \( x > 0 \) and 0 otherwise. Given \( K \) samples of \( R \) and \( r_i, i = 1, \cdots, N \), the sample average of the risk can be written as

\[
\frac{1}{K} \sum_{k=1}^{K} \mathbb{1}\{ R_k - \sum_{i=1}^{N} r_{ik} x_i > 0 \}. \tag{4.1}
\]

**Cardinality-free Models.** Let the function in (4.1) be the objective function. We can formulate the following cardinality-free nonconvex model:

\[
\min_x f(x) := \frac{1}{K} \sum_{k=1}^{K} \mathbb{1}\{ R_k - \sum_{i=1}^{N} r_{ik} x_i > 0 \}
\]

s.t. \( \sum_{i=1}^{N} x_i \leq 1 \),

\[
x_i \geq 0, \ i = 1, \cdots, N. \tag{Card-Free-Nonconvex}
\]
Using the Conditional-Value-at-Risk approximation, we can also transform the above nonconvex model into a convex one (see Appendix A.5.1 for more details):

\[
\min_{u,x} f(x,u) := u + \frac{1}{\alpha K} \sum_{k=1}^{K} \left[ -u + R_k - \sum_{i=1}^{N} r_{ik} x_i \right]_+
\]

\[
\text{s.t. } \sum_{i=1}^{N} x_i \leq 1, \quad x_i \geq 0, \quad i = 1, \ldots, N, \quad u \leq u \leq \bar{u}.
\]

(Card-Free-Convex)

**Cardinality-constrained Models.** In practice, decision makers intend to select only a portion of the available assets due to restrictions arising from transaction costs, budget constraints, etc. Such cardinality requirement can be included using the sparsity constraint \(\sum_{i=1}^{N} \mathbb{1}\{x_i > 0\} - \Psi \leq 0\), where \(\Psi\) is a given number of allowed selected assets. We can also derive its convex approximation as

\[
\sum_{i=1}^{N} v + \Psi^{-1}[x_i - v]_+ \leq 0, \quad v \leq v \leq \bar{v}.
\]

(4.2)

For the cardinality-constrained portfolio selection problem, we develop the following convex and nonconvex models:

1. Incorporate (4.2) in (Card-Free-Convex)
   (Card-Convex)

2. Incorporate constraint (4.2) in (Card-Free-Nonconvex)
   (Card-Nonconvex-1)

3. Add a weighted objective term \(\frac{1}{\Psi} \sum_{i=1}^{N} \mathbb{1}\{x_i > 0\}\) in (Card-Free-Nonconvex)
   (Card-Nonconvex-2)

Although the aforementioned convex and nonconvex models (with and without cardinality constraint) have different objective functions, the true objective is the risk in (4.1). Therefore, to evaluate the effectiveness and compare the performance of different algorithms, we focus on the value of (4.1) and the number of selected assets (mainly for cardinality-constrained models) computed by the algorithms.

**4.1.2. Tests on Stock Market Dataset** To evaluate the proposed algorithms, we test the cardinality-free and cardinality-constrained models from Section 4.1.1 using the historical stock data from six major stock markets provided by Thomson Reuters Datastream and Fama & French Data Library. The dataset contains weekly returns \(\{r_{ik}\}\) for \(N\) assets and market indices (target level) \(\{R_k\}\) across \(K\) weeks. In the original dataset, the value of \(\Psi\) for the cardinality constraint is not available. We construct it by the following rule: \(\Psi = \lfloor 0.2 \times N \rfloor\) if \(N \leq 100\) and \(\Psi = \lfloor 0.05 \times N \rfloor\)
Table 1  Features of the stock market dataset.

| Instance     | Description                  | # of assets ($N$) | # of weeks ($K$) | Cardinality ($\Psi$) |
|--------------|------------------------------|-------------------|------------------|----------------------|
| DJ           | Dow Jones Industrial Average (USA) | 28                | 1363             | 5                    |
| FF49         | Fama and French 49 Industry (USA) | 49                | 2325             | 9                    |
| ND100        | NASDAQ 100 (USA)             | 82                | 596              | 16                   |
| FTSE100      | FTSE 100 (UK)                | 83                | 717              | 16                   |
| SP500        | S&P 500 (USA)                | 442               | 595              | 22                   |
| NDComp       | NASDAQ Composite (USA)       | 1203              | 685              | 60                   |

if $N > 100$. Table 1 lists some key information about the six datasets and we refer to (Bruni et al. 2016) for more details.

In all experiments, to implement the proposed algorithms, we employ a nonconvex smooth approximation of the step functions in the objective of (Card-Free-Nonconvex) and (Card-Nonconvex-2) (see Appendix A.5.1). The initial values of $x_i$ are set to zero. In the tables below, we use the following notations: (1) “$f(x_N)$” stands for the objective value and “$\|h(x_N)\|_2$” for the norm of the cardinality constraint violation ($\sum_{i=1}^{N} x_i - \Psi$); (2) “Risk” is the value in (4.1) (it is the same as $f(x_N)$ in the nonconvex models); (3) “# ass.” represents the number of selected assets, i.e. the number of $\{x_i\}$ that are nonzero; (4) “Card vio.” records the values of cardinality violation such that Card. vio. = max(# ass. − $\Psi$, 0); (5) “Time(s)” is the CPU time in seconds.

Results of Cardinality-free Models. Table 2 and Table 3 report the computational results of applying LCG, DNCG and IPP-LCG to solve the cardinality-free models. All algorithms are terminated when the number of iteration reaches 100. In particular, for LCG and IPP-LCG, the number of iterations is the total iterations to run CGO. To examine the sparsity of the solutions, we record the values of cardinality violation, although no cardinality control is imposed in this case. From these tables, we observe that LCG, DNCG and IPP-LCG solve the models efficiently and yield relatively small risk. Without cardinality control, however, the numbers of selected assets returned by all these algorithms are larger than the required cardinality $\Psi$.

Table 2  Results of solving model (Card-Free-Convex) by LCG.

| Instance | $f(x_N)$ | Risk   | # ass. | Card. vio. | Time (s) |
|----------|----------|--------|--------|------------|----------|
| DJ       | 0.0102   | 0.0168 | 28     | 23         | 0.0262   |
| FF49     | 0.0021   | 0.0082 | 45     | 36         | 0.0485   |
| ND100    | 0.0057   | 0.0184 | 51     | 35         | 0.023    |
| FTSE100  | 0.0063   | 0.0181 | 46     | 30         | 0.025    |
| SP500    | 0.0063   | 0.0185 | 66     | 44         | 0.0412   |
| NDComp   | 0.0162   | 0.0292 | 83     | 23         | 0.141    |
Table 3  Results of solving model (Card-Free-Nonconvex) by DNCG and IPP-LCG.

| Instance | DNCG | IPP-LCG |
|----------|------|---------|
|          | Risk($f(x_N)$) | # ass. | Card. vio. | Time (s) | Risk($f(x_N)$) | # ass. | Card. vio. | Time (s) |
|DJ        | 0.019 | 27 | 22 | 0.0159 | 0.0183 | 27 | 22 | 0.0383 |
|FF49      | 0.0077 | 48 | 39 | 0.0367 | 0.0082 | 43 | 34 | 0.0588 |
|ND100     | 0.0167 | 48 | 32 | 0.0179 | 0.0184 | 51 | 35 | 0.0165 |
|FTSE100   | 0.0139 | 50 | 34 | 0.0161 | 0.0153 | 48 | 32 | 0.0255 |
|SP500     | 0.0151 | 63 | 41 | 0.0322 | 0.0067 | 81 | 59 | 0.047 |
|NDComp    | 0.0204 | 78 | 18 | 0.1557 | 0.0219 | 72 | 12 | 0.186 |

Results of Cardinality-constrained Models. For the developed cardinality-constrained models in Section 4.1.1, we solve them by LCG, DNCG and IPP-LCG, respectively, and report the numerical results in Table 4 - 6 accordingly. Intuitively, when restricting to a small pool of assets, the risk of not reaching the market index increases. As shown in Table 4 - 6, the risk (4.1) is higher than the one from the cardinality-free models (see Table 2 - 3). Nevertheless, with the cardinality constraint, all algorithms select a much smaller number of assets in a similarly efficient manner. Comparing all three algorithms, the nonconvex methods meet the cardinality requirement more strictly than their convex counterpart while the DNCG method applied on model (Card-Nonconvex-2) meet the cardinality requirement for all the instances and consumes the least CPU time for most of the instances.

Table 4  Results of solving model (Card-Convex) by LCG.

| Instance | $f(x_N)$ | $\|h(x_N)\|_2$ | Risk | # ass. | Card. vio. | Time (s) |
|----------|----------|----------------|------|--------|----------|----------|
|DJ        | 0.0429   | 0.1029         | 0.1056 | 10     | 5        | 0.0467   |
|FF49      | 0.0445   | 0.0717         | 0.248  | 13     | 4        | 0.0758   |
|ND100     | 0.0306   | 0.0423         | 0.1208 | 22     | 6        | 0.0578   |
|FTSE100   | 0.0223   | 0.0344         | 0.0586 | 22     | 6        | 0.0423   |
|SP500     | 0.0253   | 0.0296         | 0.1076 | 28     | 6        | 0.0656   |
|NDComp    | 0.0257   | 0       | 0.0175 | 60     | 0        | 0.266    |

Table 5  Results of solving model (Card-Nonconvex-1) by IPP-LCG.

| Instance | IPP-LCG |
|----------|---------|
|          | Risk($f(x_N)$) | $\|h(x_N)\|_2$ | # ass. | Card. vio. | Time (s) |
|DJ        | 0.1012   | 0.0844         | 8     | 3       | 0.0509   |
|FF49      | 0.228    | 0.0559         | 12    | 3       | 0.0801   |
|ND100     | 0.0586   | 0.0264         | 20    | 4       | 0.059    |
|FTSE100   | 0.1158   | 0.0401         | 20    | 4       | 0.0443   |
|SP500     | 0.1042   | 0.018          | 28    | 6       | 0.0777   |
|NDComp    | 0.0146   | 0               | 59    | 0       | 0.349    |
Finally, we apply the CoexDurCG algorithm proposed in (Lan et al. 2021) to solve model (Card-Convex) and report the results in Table 7. Compared with LCG (see Table 4), for instances with smaller asset pool such as “DJ”, “FF49” and “ND100”, CoexDurCG returns higher risk and selects more assets than LCG; for instances with larger pool such as “FTSE100” “SP500” and “NDComp”, CoexDurCG produces sparser solutions with less cardinality violation but the computed risk is higher and consumes more CPU time.

### Table 6
Results of solving model (Card-Nonconvex-2) by DNCG.

| Instance   | DNCG Risk($f(x_N)$) | # ass. | Card. vio. | Time (s) |
|------------|----------------------|--------|------------|----------|
| DJ         | 0.1071               | 5      | 0          | 0.0293   |
| FF49       | 0.206                | 8      | 0          | 0.0361   |
| ND100      | 0.0872               | 15     | 0          | 0.0174   |
| FTSE100    | 0.0516               | 16     | 0          | 0.0202   |
| SP500      | 0.0756               | 21     | 0          | 0.0547   |
| NDComp     | 0.0365               | 58     | 0          | 0.326    |

### Table 7
Results of solving model (Card-Convex) by CoexDurCG.

| Instance   | CoexDur CG Iter. f($x_N$) $\|h(x_N)\|_2$ Risk # ass. Card. vio. Time (s) |
|------------|---------------------------------|---------------------------------|----------------|----------------|----------------|
| DJ         | 100 0.0569 0.0559 0.1079 13 8 0.0443 |
| FF49       | 100 0.0483 0.0716 0.275 11 2 0.1189 |
| ND100      | 100 0.0473 0.0295 0.1644 22 6 0.0444 |
| FTSE100    | 100 0.0425 0.0198 0.1074 12 0 0.06658 |
|            | 150 0.0379 0.0159 0.09903 16 0 0.08253 |
| SP500      | 100 0.0396 0.0088 0.1143 9 0 0.0693 |
|            | 500 0.027 0.0072 0.0891 17 0 0.4889 |
| NDComp     | 100 0.0364 0.0017 0.0788 26 0 0.162 |
|            | 500 0.0211 0.0021 0.0365 43 0 0.6148 |
|            | 1000 0.0169 0.0018 0.0219 57 0 0.968 |

### 4.2. IMRT Treatment Planning

In this section, we first overview the IMRT treatment planning problem and formulate it as convex or nonconvex models. We then test the performance of LCG and DNCG for solving these models on four randomly generated data instances and one real-world dataset obtained from the Prostate database (https://github.com/cerr/CERR/wiki).

#### 4.2.1. Models

During the radiation therapy treatment, a patient receives prescribed radiation doses from a linear accelerator (linac), which is comprised of a set of angles ($a \in A$) and in each angle, different apertures ($e \in E_a$) can be formed to determine the doses intensity. The decisions of
the treatment planning problem consist of the selection of a set of angles and apertures as well as the determination of the doses intensity, in an effort to deliver a certain level of radiation to the tumor tissues and avoid overdoses on the healthy ones.

A desirable treatment plan operates only on a small number of angles in order to reduce the operation time. To serve the purpose, a group sparsity constraint (parameterized on $\Phi > 0$) is included as proposed in (Lan et al. 2021) in the optimization model:

$$\sum_{a \in A} \max_{e \in E_a} y_{a,e} \leq \Phi,$$

(4.3)

where $y_{a,e}$ are decision variables of intensity rate of the selected aperture $e$. Moreover, it is crucial to satisfy the required clinical criteria on particular body structures (mathematically discretized into small voxels). For instance, in the Prostate dataset,

- **underdose criteria** “PTV68: V68 $\geq 95\%$”: the percentage of voxels in structure PTV68 that receive at least 68 Gy dose should be at least 95%;
- **overdose criteria** “PTV68: V74.8 $\leq 10\%$”: the percentage of voxels in structure PTV68 that receive more than 74.8 Gy dose should not be over 10%.

A conventional way to model the clinical criteria is by risk averse constraints, in an attempt to avoid underdose (resp. overdose) to tumor (resp. healthy) structures. To be more precise, let $X$ be the random variable that denotes the amount of radiation received by certain structure. For some properly chosen right hand side $b$, the underdose/overdose criteria can be modeled by

$$\sup \{\tau : P(X < \tau) \leq \alpha\} \geq b,$$  \hspace{1cm} (underdose) \hspace{1cm} (4.4)  

$$\inf \{\tau : P(X > \tau) \leq \alpha\} \leq b.$$  \hspace{1cm} (overdose) \hspace{1cm} (4.5)

**Convex Formulation.** We refer to (Lan et al. 2021) for the convex formulation of the problem (see also Appendix A.5.2). We employ the CVaR measure to approximate (4.4) and (4.5) and obtain a convex model. However, in this formulation, more decision variables (e.g. $\tau_k$) and parameters (e.g. $b_k$) are needed to refine the approximation, to which the solutions could be very sensitive.

**Nonconvex Formulation.** To alleviate the side effects caused by the convex approximation, we attempt to formulate the objective function using (4.4) and (4.5) directly. Specifically, we minimize the weighted sample average of $P(X > \tau)$ for overdose criteria and $P(X < \tau)$ for underdose criteria. The nonconvex model uses the original clinical criteria in the objective while subjecting to the group sparse constraint (4.3) (see Appendix A.5.2 for more details).
4.2.2. Tests on Synthetic Dataset  We compare the performance of CoexDurCG and LCG applied on the convex formulation ($\Phi = 0.005$ in (4.3)) using the synthetic datasets (see Appendix A.5.3) and report the results in Table 8. In this table, the primal variable is denoted by $x_N$ and the vector of constraints by $h(x_N) = (h_s; h_c)$, including the CVaR constraints $h_c$ (for clinical criteria) and the group sparsity constraint $h_s$. We see that both algorithms consume similar CPU time to run 1000 iterations. This is expected as they are projection-free type algorithms and not required to compute full gradients of potentially high-dimensional decision variables. Besides, over all instances, both algorithms return similar objective values. However, CoexDurCG returns a solution that results in larger constraint violation, especially in the clinical constraints. We also provide numerical results of running LCG on various $\Phi$ in Appendix A.5.4.

| Instance | CoexDurCG | LCG |
|----------|-----------|-----|
|          | $f(x_N)$  | $\|h(x_N)\|_2$ | $\|h_s\|_2$ | $\|h_c\|_2$ | Time (s) | $f(x_N)$  | $\|h(x_N)\|_2$ | $\|h_s\|_2$ | $\|h_c\|_2$ | Time (s) |
| 1        | 0.0193    | 0.984 | 0.641 | 0.747 | 926 | 0.0193 | 0.528 | 0.421 | 0.319 | 924 |
| 2        | 0.0166    | 1.643 | 0.614 | 1.524 | 996 | 0.019  | 0.763 | 0.402 | 0.649 | 908 |
| 3        | 0.0467    | 1.043 | 0.205 | 1.023 | 4889 | 0.047  | 0.476 | 0.169 | 0.445 | 434 |
| 4        | 0.0465    | 3.193 | 0.208 | 3.186 | 4867 | 0.0435 | 0.984 | 0.175 | 0.968 | 4871 |

4.2.3. Tests on Prostate Dataset  In this part, we conduct numerical experiments on a publicly available dataset of a patient with prostate cancer. The dataset has 3,047,040 voxels and 180 angles, with the granularity of beamlets grids (beamlet unit length) equal to 1.0 for each angle. The average number of beamlets is 155. As such, the dimension of the data matrices reaches more than 3,047,040 × 155 × 180. More importantly, the dataset contains 10 clinical criteria for six structures: PTV56: $V_{56} \geq 95\%$; PTV68: $V_{68} \geq 95\%$, $V_{74.8} \leq 10\%$; Rectum: $V_{30} \leq 80\%$, $V_{50} \leq 50\%$, $V_{65} \leq 25\%$; Bladder: $V_{40} \leq 70\%$, $V_{65} \leq 30\%$; Left femoral head: $V_{50} \leq 1\%$; Right femoral head: $V_{50} \leq 1\%$. In our numerical study, the obtained solution is evaluated by whether it satisfies all above the clinical criteria.

This IMRT problem with Prostate dataset is notoriously difficult for the following challenges.

First, the aforementioned clinical criteria inherit potential contradiction. For example, the tumor structure “PTV68” and the healthy structures “Bladder” and “Rectum” are very close, but it is required that at least 95% of the tumor structure receives no less than 68 Gy dose while strict percentage cap is placed on the dose received by the healthy ones.

Second, it is tricky to meet the underdose and overdose clinical criteria simultaneously for the “PTV68” structure. To see this, the difference between the upper dose limit (74.8 Gy) and the
lower dose limit (68 Gy) is very close, which implies that one necessary condition to satisfy the underdose and overdose criteria is that at least 90% of the received dose should fall in [68, 74.8].

Third, in order to shorten the operation time, we need to select small number of angles with no more than 100 apertures in total. Such requirements are potentially conflicting with accomplishing the target of dose delivery. Therefore, the model and algorithms should be designed to make smart trade-offs.

Last, the dimension of the data matrices are over 3 million \(\times\) 155 \(\times\) 180, leading to high dimensional decision space with potential size larger than 180 \(\times\) 45\(^10\), which is quite computationally cumbersome, and prevents any methods requiring full gradient computation.

Results of the Convex Formulation. We apply the LCG algorithm to solve the convex formulation. In Table 9, we summarize the treatment plan (number of angles, number of apertures) constructed by LCG and the number of iterations needed to deliver the plan. From the table, we see that when \(\Phi\) is smaller, the algorithm tends to select less angles, which is an expected effect of the group sparsity constraint.

| \(\Phi\) | # of iter. | # of angels | # of apertures |
|---------|------------|-------------|----------------|
| 1.0     | 100        | 27          | 99             |
| 0.5     | 85         | 17          | 84             |
| 0.005   | 63         | 6           | 62             |
| 0.0005  | 78         | 5           | 77             |

Table 10 details the fulfillment of the clinical criteria for different sparsity parameters \(\Phi\). Here in the table, each column (starting from the second one) represents the clinical criteria (criterion) of particular structure. For each of them (e.g. PTV68 / V68\(\geq\) 95%), the first line (e.g. PTV68) indicates the treated structure; in the second line (and onwards), take “V68\(\geq\) 95%” as an instance, it means that the percentage of voxels that receive at least 68 Gy dose (V68) should be no less than 95% (\(\geq\) 95%); in the instance of “V74.8\(\leq\) 10%”, it means that the percentage of voxels that receive more than 74.8 Gy dose (V74.8) should be no larger than 10% (\(\leq\) 10%). In each line at each cell of the table, we record such voxel percentages correspondingly computed by the algorithm. In the case of “V68\(\geq\) 95%”, when the recorded value is no less than 0.95, then the clinical criterion “PTV68 / V68\(\geq\) 95%” is satisfied; in the case of “V74.8\(\leq\) 10%”, when the recorded value is no larger than 0.1, then the clinical criterion “PTV68 / V74.8\(\leq\) 10%” is satisfied.

From the displayed results in Table 10, when \(\Phi = 0.005\), the algorithm returns fairly good solution in terms of satisfying all clinical criteria, except for the criterion PTV68: V74.8 \(\leq\) 10%. Combining the results in both Table 9 and 10, we find that when \(\Phi = 0.005\), the algorithm yields the best results with respect to the number of selected angles and the satisfaction of the clinical criteria.
Table 10    Results of applying LCG on Prostate dataset.

| Φ         | PTV56 V65 ≥ 95% | PTV68 V68 ≥ 95% | Rectum V30 ≤ 80% | Bladder V40 ≤ 70% | Lft. femoral head V50 ≤ 50% | Rht. femoral head V65 ≤ 30% |
|-----------|----------------|----------------|------------------|-------------------|-----------------------------|-----------------------------|
|           | V74.8 ≤ 10%    | V50 ≤ 50%      | V50 ≤ 1%         | V50 ≤ 1%          |                             |                             |
| 1.0       | 0.9997         | 0.9647         | 0.6825           | 0.5365            | 0.0011                      | 0.001                       |
|           | 0.1593         | 0.2188         | 0.2179           | 0.0601            |                             |                             |
| 0.5       | 0.9966         | 0.9536         | 0.7126           | 0.5239            | 0.01                        | 0.0023                      |
|           | 0.1423         | 0.2455         | 0.2115           | 0.0533            |                             |                             |
| 0.005     | 0.9987         | 0.9544         | 0.7778           | 0.552             | 0.0024                      | 0.0                          |
|           | 0.1263         | 0.3786         | 0.2287           | 0.0561            |                             |                             |
| 0.0005    | 0.9994         | 0.9056         | 0.7998           | 0.6198            | 0.0003                      | 0.0022                      |
|           | 0.1151         | 0.3804         | 0.2556           | 0.1071            |                             |                             |

Results of the Nonconvex Formulation. We apply the DNCG method to solve the nonconvex formulation. In this case, the sparsity parameter Φ is set to be 0.005 provided that it demonstrates the best numerical performance in the convex case. We provide two types of results:

1. DNCG: run the algorithm on a set of trivially generated initial points.
2. LCG initial + DNCG: run DNCG with a set of initial solutions computed by LCG.

For implementation of “LCG initial + DNCG”, the starting point is obtained by solving the convex model with sparsity parameter Φ = 0.005 at iteration 63 (see Table 9 and 10). In this way, the initial solution is feasible in terms of satisfying all clinical criteria except for “PTV 68: V74.8 ≤ 10%”. Results of a treatment plan (selected angles/apertures) constructed by the proposed algorithms are shown in Table 11. In Table 12, we demonstrate the fulfillment of the clinical criteria by applying DNCG with two different initialization schemes as mentioned above. With the trivial initialization, the DNCG algorithm produces a solution that meets all criteria, even for the hard criterion “PTV 68: V74.8 ≤ 10%”. One downside is that it selects more angles and consumes more number of iterations, compared to the LCG algorithm. With warm-up initialization, DNCG selects less number of angles and requires less number of iterations while satisfying all clinical criteria.

Table 11    Treatment plans constructed by DNCG with different initial conditions on Prostate dataset.

| Type                  | Φ        | # of iter. | # of angels | # of apertures |
|-----------------------|----------|------------|-------------|---------------|
| DNCG                  | 0.005    | 96         | 14          | 83            |
| LCG initial + DNCG    | 0.005    | 63(convex)+17(nonconvex) | 9          | 75            |
Table 12  Results of applying DNCG and LCG initial+ DNCG on Prostate dataset.

| Type       | Φ  | PTV56 |     | PTV68 |     | Rectum |     | Bladder |     | Lft. femoral head |     | Rht. femoral head |     |
|------------|----|-------|-----|-------|-----|--------|-----|---------|-----|-------------------|-----|-------------------|-----|
|            |    | V56≥95% |     | V68≥95% |     | V30≤80% |     | V40≤70% |     | V50≤50%          |     | V65≤30%          |     |
|            |    | V74.8≤10% |     | V65≤25% |     | V40≤70% |     | V50≤1% |     | V50≤1%          |     |                  |     |
| DNCG       | 0.005 | 0.9522 |     | 0.9549 |     | 0.7506 |     | 0.5299 |     | 0.0012 |     | 0.0 |     |
| LCG initial |    | 0.9571 |     | 0.9503 |     | 0.7829 |     | 0.5411 |     | 0.00067 |     | 0.0 |     |
| + DNCG     | 0.005 | 0.0126 |     | 0.3844 |     | 0.2204 |     |                  |     |                  |     |     |     |

5. Conclusion

To cater for the emergent applications in risk averse sparse optimization and tackle the accompanying challenges, in this paper, we develop novel projection-free methods to solve a class of convex and nonconvex functional constrained problems. In particular, we propose the Level Conditional Gradient (LCG) method for solving the convex problems and show that the iteration complexity of the proposed algorithm solving for an ε-solution is bounded by $O(\frac{1}{\varepsilon^2} \log (\frac{1}{\varepsilon}))$. This complexity does not depend on the size of a (possibly) large Lagrange multiplier. For the nonconvex problem, we develop an Inexact Proximal Point (IPP-LCG) method, with convergence analysis revealing that the iteration complexity of searching for an $(\epsilon, \epsilon)$-KKT point is bounded by $O(\frac{1}{\epsilon^3} \log (\frac{1}{\epsilon}))$. As a remedy to the three-layer nested structure in IPP-LCG, we propose a single-loop Nonconvex Conditional Gradient (DNCG) method and show that the iteration complexity is bounded by $O(1/\epsilon^4)$ to obtain an ε-Wolfe solution. To the best our knowledge, all these theoretical results are new in the literature. We demonstrate the effectiveness of LCG, IPP-LCG and DNCG by applying them on the portfolio selection and the IMRT treatment planning problems. The numerical studies verify that all methods are computationally efficient in solving such risk averse sparse convex and nonconvex models, respectively. We also expect that the developed projection-free algorithms will find wider applications beyond sparse and risk averse optimization.

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Appendix

A.1. Convergence Analysis of CGO

A.1.1. Auxiliary Lemmas

To establish the convergence for CGO, we tap into the following three well-studied results. Throughout the analysis, we need to use the following notation: let $\alpha_t$ be defined in Algorithm 2, define the sequence $\{\Gamma_t\}$ as $\Gamma_t := \begin{cases} 1, & \text{if } t = 1, \\ (1 - \alpha_t)\Gamma_{t-1}, & \text{if } t > 1. \end{cases}$ $t = 1, 2, \ldots$

The first lemma is the so-called “three-point” lemma which characterizes the optimality condition of the dual update in (2.10).

**Lemma A.1.1.** (Lan 2020, Lemma 3.1) Let $r_t$ be defined in (2.10). Then

$$\langle -\bar{h}_t, r_t - z \rangle + \tau_t V(r_{t-1}, r_t) \leq \tau_t V(r_{t-1}, z) - \tau_t V(r_t, z), \forall z \in \bar{Z}.$$

The second lemma deals with telescoping sums.

**Lemma A.1.2.** (Lan 2020, Lemma 3.17) Let $\{R_t\}$ be some given sequence. A sequence $\{S_t\}$ such that

$$S_t \leq (1 - \alpha_t)S_{t-1} + R_t, \ t = 1, 2, \ldots,$$

satisfies

$$\frac{S_t}{\Gamma_t} \leq (1 - \alpha_1)S_0 + \sum_{j=1}^{t} \frac{R_j}{\Gamma_j}.$$

We utilize the following properties for smooth functions.

**Lemma A.1.3.** (Lan 2020, Lemma 3.2): Let $p_t, x_t$ be defined in Algorithm 2. If $\bar{f}$ and $\bar{h}$ are smooth functions such that $\forall x_1, x_2 \in X, \|\nabla \bar{f}(x_1) - \bar{f}(x_2)\| \leq L_{\bar{f}}\|x_1 - x_2\|$ and $\|\nabla \bar{h}_i(x_1) - \bar{h}_i(x_2)\| \leq L_{\bar{h}_i}\|x_1 - x_2\|, i = 1, \ldots, \bar{m}$, then the following conditions hold:

$$\bar{f}(x_t) \leq (1 - \alpha_t)\bar{f}(x_{t-1}) + \alpha_t\ell_f(x_{t-1}, p_t) + \frac{L_{\bar{f}}\alpha_t^2}{2}\|p_t - x_{t-1}\|^2,$$

$$\bar{h}_i(x_t) \leq (1 - \alpha_t)\bar{h}_i(x_{t-1}) + \alpha_t\ell_{\bar{h}_i}(x_{t-1}, p_t) + \frac{L_{\bar{h}_i}\alpha_t^2}{2}\|p_t - x_{t-1}\|^2, i = 1, \ldots, \bar{m}.$$

The lemma below establishes a lower bound of $f(x_t) - f^*$ for the convex constrained problem (1.1) since $x_t$ may not be satisfy $h(x_t) \leq 0$. 
Lemma A.1.4. Let \((x^*, y^*) \in \mathbb{R}^n \times \mathbb{R}^m\) be the saddle point of the convex constrained problem (1.1). Let \((\gamma^*, z^*)\) be the optimal dual solution of the root finding problem

\[
\min_{x \in X} \max_{(\gamma, z) \in Z} L(x, (\gamma, z)) := \gamma [f(x) - f^*] + \langle h(x), z \rangle
\]

(i.e. problem (2.1) with \(l = f^*\)). Denote \([\cdot]_+ := \max\{0, \cdot\}\). Then \(\forall x \in X, f(x) - f^*\) is lower bounded such that

\[
f(x) - f^* \geq -\min\{\|y^*\|, \|z^*\|, \frac{\|z^*\|}{\gamma^*}\} \|[h(x)]_+\|.
\]

**Proof.** According to the result in (Lan and Monteiro 2013, Corollary 2), we have

\[
f(x) - f^* \geq -\|[h(x)]_+\|.
\]  

(A.1.3)

Since \((x^*, (\gamma^*, z^*))\) is a pair of saddle point of (A.1.1), thus by the saddle point theorem, we have

\[
L(x^*, (\gamma, z)) \leq L(x^*, (\gamma^*, z^*)) \leq L(x, (\gamma^*, z^*)), \forall x \in X, (\gamma, z) \in Z.
\]

Using the above relation and the facts that \(L(x^*, (\gamma^*, z^*)) = 0, \langle [h(x)]_+ - h(x), z^* \rangle \geq 0\), we have \(\forall x \in X:\)

\[
\gamma^* [f(x) - f^*] = L(x, (\gamma^*, z^*)) - \langle h(x), z^* \rangle \leq L(x^*, (\gamma^*, z^*)) - \langle h(x), z^* \rangle \geq -\|[h(x)]_+\| \|z^*\|.
\]

(A.1.4)

Combining (A.1.3) and (A.1.4), we obtain \(\forall x \in X:\)

\[
f(x) - f^* \geq -\min\{\|y^*\|, \|z^*\|, \frac{\|z^*\|}{\gamma^*}\} \|[h(x)]_+\|.
\]

(A.1.5)

A.1.2. CGO for Smooth Functions

Lemma 2.2. Let \(\tilde{\phi}, L_t\) and \(U_t\) be defined in (2.8), (2.16) and (2.17), respectively. Also let \(z_t\) be defined in (2.11). Then we have

\[
f_t(x) \leq \tilde{f}(x),
\]

\[
h_t(x) \leq \tilde{h}(x), z_t,
\]

\[
L_t \leq \tilde{\phi} \leq U_t,
\]

for any \(t \geq 1.\)
Proof. The relation \( f_t(x) \leq \tilde{f}(x) \) immediately follows from the initial condition \( f_0(x) \leq \tilde{f}(x) \) and the fact that \( f_t(x) \) is the convex combinations of two lower bounding functions of \( \tilde{f}(x) \) by (2.14).

Let \( r_t \) be defined in (2.10). Using the relation of \( 1 - \alpha_t = \frac{\Gamma_t}{\Gamma_{t-1}} \) and dividing both sides of (2.15) by \( \Gamma_t \), we have

\[
\frac{1}{\Gamma_t} h_t(x) = \frac{1}{\Gamma_{t-1}} h_{t-1}(x) + \frac{\alpha_t}{\Gamma_t} \langle \ell_h(x_{t-1}, x), r_t \rangle \\
\leq \frac{1}{\Gamma_{t-1}} h_{t-1}(x) + \frac{\alpha_t}{\Gamma_t} \langle \tilde{h}(x), r_t \rangle \\
= \sum_{j=1}^{t} \frac{\alpha_j}{\Gamma_j} \langle \tilde{h}(x), r_j \rangle, \tag{A.1.6}
\]

where the second inequality follows from \( \ell_h(x_t, x) \leq \tilde{h}(x) \), the third inequality is due to the recursive deduction. Multiplying both sides of (A.1.6) with \( \Gamma_t \), along with the initial condition that \( h_0(x) \leq \tilde{h}(x) \), we conclude that

\[
h_t(x) \leq \langle \tilde{h}(x), \sum_{j=1}^{t} \theta_j r_j \rangle = \langle \tilde{h}(x), z_t \rangle,
\]

where \( \theta_j := \Gamma_t \frac{\alpha_j}{\Gamma_j} \) with \( \sum_{j=1}^{t} \theta_j = 1 \) and \( z_t = \sum_{j=1}^{t} \theta_j r_j \). It then follows \( f_t(x) + h_t(x) \leq \tilde{f}(x) + \langle \tilde{h}(x), z_t \rangle, \forall x \in \hat{X} \). By the definition of \( L_t \) in (2.16), we have \( L_t \leq \min_{x \in \hat{X}} \max_{z \in \hat{Z}} \tilde{f}(x) + \langle \tilde{h}(x), z \rangle \), which shows that \( L_t \) is a valid lower bound of problem (2.8). Moreover, using the fact that

\[
\forall x \in \hat{X}, \max_{z \in \hat{Z}} \tilde{f}(x) + \langle \tilde{h}(x), z \rangle \geq \min_{x \in \hat{X}} \max_{z \in \hat{Z}} \tilde{f}(x) + \langle \tilde{h}(x), z \rangle,
\]

and the definition of \( U_t \) in (2.17) and \( x_{t-1}, p_t \in \hat{X} \), we obtain

\[
U_t = \max_{z \in \hat{Z}} \tilde{f}(x_t) + \langle \tilde{h}(x_t), z \rangle \geq \min_{x \in \hat{X}} \max_{z \in \hat{Z}} \tilde{f}(x) + \langle \tilde{h}(x), z \rangle.
\]

\( \square \)

The following proposition establishes the recursion of the gap function (2.21) for CGO, which is an important intermediate step to the proof of the main theorem.

**Proposition A.1.1.** At iteration \( t > 1 \), we have

\[
Q_t(w_t, w) \leq (1 - \alpha_t) Q_{t-1}(w_{t-1}, w) + \frac{(L_{\tilde{f}} + z^\top L_{\tilde{h}}) \alpha_t^2}{2} D_{X}^2 + \frac{9 \alpha_t \lambda_t^2 M^2 D_{X}^2}{2 \tau_t} + \alpha_t [\ell_{\tilde{h}}(x_{t-1}, p_t) - \ell_{\tilde{h}}(x_{t-2}, p_{t-1}) - \ell_{\tilde{h}}(x_{t-3}, p_{t-2}) - \ell_{\tilde{h}}(x_{t-4}, p_{t-3}) - \cdots] + \alpha_t [\tau_t V(r_{t-1}, z) - \tau_t V(r_t, z)].
\]
Proof. Together by the definition of $\bar{Q}_t(w_t, w), f_t, h_t$ respectively in (2.21), (2.14) and (2.15) and Lemma A.1.3, for any $w \in \bar{X} \times \bar{Z}$, we have

\[
\bar{Q}_t(w_t, w) \leq (1 - \alpha_t) \bar{f}(x_{t-1}) + \alpha_t \ell_f(x_{t-1}, p_t) + \frac{L_f \alpha_t^2}{2} \|p_t - x_{t-1}\|^2 \\
+ (1 - \alpha_t) \langle \bar{h}(x_{t-1}), z \rangle + \alpha_t \langle \ell_h(x_{t-1}, p_t), z \rangle + \frac{z^\top L_h \alpha_t^2}{2} \|p_t - x_{t-1}\|^2 \\
- (1 - \alpha_t) \bar{f}_t(x_{t-1}, x) - (1 - \alpha_t) \bar{h}_t(x_{t-1}, x) - \alpha_t \langle \ell_h(x_{t-1}, x), r_t \rangle \\
\leq (1 - \alpha_t) \left[ \bar{f}(x_{t-1}) + \langle \bar{h}(x_{t-1}), z \rangle - \bar{f}_t(x_{t-1}, x) - \bar{h}_t(x_{t-1}, x) \right] + \frac{(L_f + z^\top L_h) \alpha_t^2}{2} D_{\bar{X}}^2 \\
+ \alpha_t \left[ \ell_f(x_{t-1}, p_t) + \langle \ell_h(x_{t-1}, p_t), z \rangle - \ell_f(x_{t-1}, x) - \langle \ell_h(x_{t-1}, x), r_t \rangle \right].
\] (A.1.7)

The primal update (2.12) implies that

\[
\ell_f(x_{t-1}, p_t) + \langle \ell_h(x_{t-1}, p_t), r_t \rangle \leq \ell_f(x_{t-1}, x) + \langle \ell_h(x_{t-1}, x), r_t \rangle, \ \forall x \in \bar{X}.
\]

Rearranging the terms in the above inequality, we have

\[
\ell_f(x_{t-1}, p_t) + \langle \ell_h(x_{t-1}, p_t), z \rangle - \ell_f(x_{t-1}, x) - \langle \ell_h(x_{t-1}, x), r_t \rangle \leq \langle \ell_h(x_{t-1}, p_t), z - r_t \rangle. \tag{A.1.8}
\]

Meanwhile, by Lemma A.1.1, we obtain

\[
\langle \ell_h(x_{t-1}, p_t), z - r_t \rangle \leq \langle \ell_h(x_{t-1}, p_t) - \bar{h}_t, z - r_t \rangle + \tau_t V(r_{t-1}, z) - \tau_t V(r_t, z) - \tau_t V(r_{t-1}, r_t). \tag{A.1.9}
\]

In addition,

\[
\langle \ell_h(x_{t-1}, p_t) - \bar{h}_t, z - r_t \rangle = \langle \ell_h(x_{t-1}, p_t) - \bar{h}_t, z - r_t \rangle - \lambda_t \langle \ell_h(x_{t-2}, p_{t-1}) - \bar{h}_t, z - r_{t-1} \rangle \\
+ \lambda_t \langle \ell_h(x_{t-2}, p_{t-1}) - \bar{h}_t, z - r_{t-1} \rangle - \lambda_t V(r_{t-1}, r_t) \\
\leq \langle \ell_h(x_{t-1}, p_t) - \bar{h}_t, z - r_t \rangle - \lambda_t \langle \ell_h(x_{t-2}, p_{t-1}) - \bar{h}_t, z - r_{t-1} \rangle \\
+ \frac{9 \lambda_t^2 M^2 D_{\bar{X}}^2}{2 \tau_t},
\] (A.1.10)

where the first equality follows from the definition of $\bar{h}_t$ in (2.9) and the last inequality is due to

\[
\lambda_t \langle \ell_h(x_{t-2}, p_{t-1}) - \bar{h}_t, z - r_{t-1} \rangle - \tau_t V(r_{t-1}, r_t) \\
\leq \frac{\lambda_t^2}{2 \tau_t} \| \ell_h(x_{t-2}, p_{t-1}) - \bar{h}_t, z - r_{t-1} \| \| z - r_{t-1} \|^2 \\
= \frac{\lambda_t^2}{2 \tau_t} \| \bar{h}(x_{t-2}) - \bar{h}(x_{t-3}) + (\nabla \bar{h}(x_{t-2}), p_{t-1} - x_{t-2}) + (\nabla \bar{h}(x_{t-3}), x_{t-3} - p_{t-2}) \| \| z - r_{t-1} \|^2 \\
\leq \frac{\lambda_t^2}{2 \tau_t} \| \bar{h}(x_{t-2}) - \bar{h}(x_{t-3}) + \bar{h}(p_{t-1}) - \bar{h}(x_{t-2}) + \bar{h}(p_{t-2}) - \bar{h}(x_{t-3}) \| \| z - r_{t-1} \|^2 \\
\leq \frac{9 \lambda_t^2 M^2 D_{\bar{X}}^2}{2 \tau_t}. \tag{A.1.11}
\]

Plugging (A.1.8), (A.1.9) and (A.1.10) into (A.1.7), we prove the result. \qed
Proposition A.1.2. Suppose for \( t \geq 2 \), parameters \( \{\alpha_t\}, \{\lambda_t\} \) and \( \{\tau_t\} \) in Algorithm 2 satisfy
\[
\alpha_1 = 1, \quad \frac{\lambda_t \alpha_t}{\Gamma_t} = \frac{\alpha_t - 1}{\Gamma_t - 1} \text{ and } \frac{\alpha_t \tau_t}{\Gamma_t} \geq \frac{\alpha_t - 1}{\Gamma_t - 1} \tag{A.1.12}
\]
Then for the general saddle point problem (2.8), for \( T \geq 1 \), we have
\[
Q_T(w_T, w) \leq \Gamma_T T \sum_{t=1}^{T} \left[ \frac{(L_f^T + z^T L_h)\alpha_t^2}{2\Gamma_t} D^2 + \frac{9\alpha_t \lambda_t^2 M^2 D^2}{2\tau_t \Gamma_t} \right] + \frac{9\alpha_T M^2 D^2}{2\tau_T} + \alpha_T \tau_T V, \tag{A.1.13}
\]
\( \forall w \in \bar{X} \times \bar{Z} \).

Proof. In view of Lemma A.1.2 and Proposition A.1.1 as well as \( 1 - \alpha_1 = 0 \), we have
\[
\frac{\bar{Q}_T(w_T, w)}{\Gamma_T} \leq \sum_{t=1}^{T} \left[ \frac{(L_f^T + z^T L_h)\alpha_t^2}{2\Gamma_t} D^2 + \frac{9\alpha_t \lambda_t^2 M^2 D^2}{2\tau_t \Gamma_t} \right] + \sum_{t=1}^{T} \frac{\alpha_t \tau_t}{\Gamma_t} \left[ (\ell_h(x_{t-1}, p_t) - \ell_h(x_{t-2}, p_{t-1}), z - r_t) - \lambda_t (\ell_h(x_{t-2}, p_{t-1}) - \ell_h(x_{t-3}, p_{t-2}), z - r_{t-1}) \right] + \sum_{t=1}^{T} \frac{\alpha_t \tau_t}{\Gamma_t} \left[ V(r_{t-1}, z) - V(r_t, z) \right], \forall w \in \bar{X} \times \bar{Z}.
\]
The second equation in (A.1.12) indicates that summing up the extrapolated linear function values from 1 to \( T \) cancels out intermediate terms, such that
\[
\sum_{t=1}^{T} \frac{\alpha_t \tau_t}{\Gamma_t} \left[ (\ell_h(x_{t-1}, p_t) - \ell_h(x_{t-2}, p_{t-1}), z - r_t) - \lambda_t (\ell_h(x_{t-2}, p_{t-1}) - \ell_h(x_{t-3}, p_{t-2}), z - r_{t-1}) \right]
= \alpha_T (\ell_h(x_{T-1}, p_T) - \ell_h(x_{T-2}, p_{T-1}), z - r_T) - \lambda_T (\ell_h(x_{T-2}, p_{0}) - \ell_h(x_{T-3}, p_{-1}), z - r_{0}).
\]

Besides, the third inequality in (A.1.12) implies
\[
\sum_{t=1}^{T} \frac{\alpha_t \tau_t}{\Gamma_t} \left[ V(r_{t-1}, z) - V(r_t, z) \right]
= \frac{\alpha_1 \tau_1}{\Gamma_1} V(r_0, z) + \sum_{t=2}^{T} \left( \frac{\alpha_t \tau_t}{\Gamma_t} - \frac{\alpha_{t-1} \tau_{t-1}}{\Gamma_{t-1}} \right) V(r_{t-1}, z) - \frac{\alpha_T \tau_T}{\Gamma_T} V(r_T, z)
\leq \frac{\alpha_1 \tau_1}{\Gamma_1} \tilde{V} + \sum_{t=2}^{T} \left( \frac{\alpha_t \tau_t}{\Gamma_t} - \frac{\alpha_{t-1} \tau_{t-1}}{\Gamma_{t-1}} \right) \tilde{V} - \frac{\alpha_T \tau_T}{\Gamma_T} V(r_{T-1}, z)
\leq \frac{\alpha_T \tau_T}{\Gamma_T} \tilde{V} - \frac{\alpha_T \tau_T}{\Gamma_T} V(r_T, z).
\tag{A.1.14}
\]

Using the above relations, together with the initial condition \( x_{-2} = x_{-1}, \ p_{-1} = p_{0} \) which gives \( \ell_h(x_{-1}, p_{0}) - \ell_h(x_{-2}, p_{-1}) = 0 \) and the relation that
\[
\alpha_T (\ell_h(x_{T-1}, p_T) - \ell_h(x_{T-2}, p_{T-1}), z - r_T) - \alpha_T \tau_T V(r_T, z) \leq \frac{9M^2 \alpha_T D^2}{2\tau_T},
\]
we conclude that \( \forall w \in X \times Z \),

\[
\bar{Q}_T(w_T, w) \leq \Gamma_T \sum_{t=1}^{T} \left[ \frac{(L_f + z^T L_h)\alpha_t^2 D_X^2}{2\Gamma_t} + \frac{9\alpha_t\lambda_t^2 M^2 D_X^2}{2\tau_t\Gamma_t} \right] + \alpha_T \tau_T V(\ell_T, w) - \bar{\ell}_h(\ell_H, z) - \bar{\ell}_h(\ell_H, z) - \lambda_h(\ell_h, \lambda_h, z) - \lambda_h(\ell_h, \lambda_h, z) + \alpha_T \tau_T \bar{V}.
\]

We will specify the parameters \( \{\alpha_t, \lambda_t, \tau_t\} \) in Algorithm 2. We will also demonstrate that the selected parameters \( \{\tau_t\} \) does not depend on the number of iteration \( T \).

**Theorem 2.2** Suppose that the algorithmic parameters in CGO are set to

\[
\alpha_t = \frac{2}{t+1}, \quad \lambda_t = \frac{t-1}{t}, \quad \tau_t = 9\sqrt{tM}D_X, t \geq 1.
\]

Then for any \( t \geq 1 \),

\[
\bar{Q}_t(w_t, w) \leq \frac{2(L_f + z^T L_h)D_X^2}{t+1} + \frac{MD_X}{\sqrt{t+1}} \left[ 18\bar{V} + \frac{7}{6} \right] \forall w \in (\bar{X}, \bar{Z}).
\]

**Proof.** It is easy to verify that the identities in (2.22) satisfy the conditions in (A.1.12). By definition of \( \{\alpha_t\} \) and \( (2.22) \), we have \( \Gamma_t = \frac{2}{t(t+1)} \) and \( \alpha_t/\Gamma_t = t \), so that for any \( T \geq 1 \)

\[
\Gamma_T \sum_{t=1}^{T} \frac{\alpha_t^2}{2\Gamma_t} = \Gamma_T \sum_{t=1}^{T} \frac{t}{t+1} \leq \frac{2}{T+1},
\]

\[
\Gamma_T \sum_{t=1}^{T} \frac{9\alpha_t\lambda_t^2}{2\tau_t\Gamma_t} \leq \frac{2\sqrt{T}}{3(T+1)MD_X}.
\]

Plugging the above relations in (A.1.13), we obtain

\[
\bar{Q}_T(w_T, w) \leq \frac{2(L_f + z^T L_h)D_X^2}{T+1} + \frac{2\sqrt{TMD_X}}{3(T+1)} + \frac{MD_X}{\sqrt{T(T+1)} + 18\sqrt{TMD_X}V}
\]

\[
= \frac{2(L_f + z^T L_h)D_X^2}{T+1} + \frac{MD_X}{\sqrt{T(T+1)} + 18\sqrt{TMD_X}V}
\]

\[
\leq \frac{2(L_f + z^T L_h)D_X^2}{T+1} + \frac{MD_X}{\sqrt{T+1}} \left[ 18\bar{V} + \frac{7}{6} \right], \forall w \in (\bar{X}, \bar{Z}).
\]

In this way, we show the conclusion in (2.23).
A.1.3. CGO for Structured Nonsmooth Functions

In this section, we focus on problem (2.8) where \( \tilde{f}(\cdot) \) and \( \bar{h}_i(\cdot), \ i = 1, \cdots, \bar{m} \) are structured nonsmooth functions represented by the following form (see also Nesterov (2005)):

\[
\tilde{f}(x) = \max_{y \in Y_0} \{ \langle B_0 x, y \rangle - \tilde{f}(y) \}, \tag{A.1.18}
\]

\[
\bar{h}_i(x) = \max_{y \in Y_i} \{ \langle B_i x, y \rangle - \bar{h}_i(y) \}, \ i = 1, \cdots, \bar{m},
\]

where \( Y_i, \ i = 1, \cdots, \bar{m} \) are closed convex sets, \( \tilde{f} \) and \( \bar{h}_i \) are simple (continuous and differentiable) convex functions, possibly \( \omega_i \)-strongly convex \( i = 0, 1, \cdots, \bar{m} \). Let \( u_i : Y_i \to \mathbb{R} \) be a 1-strongly convex distance generating function. Define the proximal function \( U_i \) as \( U_i(x) := u_i(y) - u_i(y_i) - \langle \nabla u_i(y_i), y - y_i \rangle, \ y \in Y_i \), where \( y_i := \arg \min_{y \in Y} u_i(y) \). Further let \( \eta_i, \ i = 0, \cdots, \bar{m} \) be the smoothing parameters that can vary or stay static over iterations.

To generalize CGO to solve problems with structured nonsmooth functions, we need to leverage the Nesterov smoothing scheme (Nesterov 2005) to approximate the possibly nonsmooth functions \( \tilde{f} \) and \( \bar{h}_i \) by \( \tilde{f}_{0\eta_0} \) and \( \bar{h}_{i\eta_i} \) stated below:

\[
\tilde{f}_{0\eta_0}(x) := \max_{y \in Y_0} \{ \langle B_0 x, y \rangle - \tilde{f}(y) - \eta_0 U_0(y) \}, \tag{A.1.16}
\]

\[
\bar{h}_{i\eta_i}(x) := \max_{y \in Y_i} \{ \langle B_i x, y \rangle - \bar{h}_i(y) - \eta_i U_i(y) \}, \ i = 1, \cdots, \bar{m}. \tag{A.1.17}
\]

It can be shown that (see Nesterov (2005)), \( \tilde{f}_{0\eta_0} \) and \( \bar{h}_{i\eta_i} \) are differentiable with Lipschitz constants \( L \tilde{f}_{0\eta_0} := \frac{\|B_0\|^2}{\omega_0 + \eta_0} \) and \( L \bar{h}_{i\eta_i} := \frac{\|B_i\|^2}{\omega_i + \eta_i} \). Suppose \( Y_i, i = 1, \cdots, \bar{m} \) are compact, then \( \bar{h}_{i\eta_i} \) have bounded gradients such as \( \|\nabla h_{i\eta_i}(x)\|_{\infty} \leq \tilde{M}_{B_i, U_i}, \) where \( \tilde{M}_{B_i, U_i} := \|B_i\|\left(\|y_i\| + \sqrt{2D_i}\right), \ i = 1, \cdots, \bar{m}, \ D_i := \left(\max_{y \in Y_i} U_i(y)\right) \). Moreover, the relation between the original functions and the smoothing counterparts are characterized by

\[
\tilde{f}_{0\eta_0}(x) \leq \tilde{f}(x) \leq \tilde{f}_{0\eta_0}(x) + \eta_0 D^2_{U_0}, \tag{A.1.18}
\]

\[
\bar{h}_{i\eta_i}(x) \leq \bar{h}_i(x) \leq \bar{h}_{i\eta_i}(x) + \eta_i D^2_{U_i}, \ i = 1, \cdots, \bar{m}.
\]

In this part, we focus on the case where the smoothing parameters \( \eta_i, \ i = 0, 1, \cdots, \bar{m} \) are adapted over iterations such as

\[
\eta_0^0 \geq \eta_1^1 \geq \cdots \geq \eta_i^i, \ i = 0, 1, \cdots, \bar{m}. \tag{A.1.19}
\]

In this case, at each iteration \( t \), the approximations of \( \tilde{f} \) and \( \bar{h} \) are \( \tilde{f}_{0\eta_0} \) and \( \bar{h}_{i\eta_i} \). Accordingly, their Lipschitz constants are changed to \( L \tilde{f}^t := L \tilde{f}_{0\eta_0} := \frac{\|B_0\|^2}{\omega_0 + \eta_0^t} \) and \( L \bar{h}_i^t := L \bar{h}_{i\eta_i} := \frac{\|B_i\|^2}{\omega_i + \eta_i^t} \). Nevertheless, the relation in (A.1.18) still holds for each \( \bar{f}_{0\eta_0} \) and \( \bar{h}_{i\eta_i} \) at iteration \( t \). Moreover, similar to (Lan et al. 2021), it can be shown that the sequences \( \{\tilde{f}_{0\eta_0}^t\}_t \) and \( \{\bar{h}_{i\eta_i}^t\}_t \) satisfy:

\[
\tilde{f}_{0\eta_0}^{t-1} \leq \tilde{f}_{0\eta_0}^t \leq \tilde{f}_{0\eta_0}^{t-1} + (\eta_0^{t-1} - \eta_0^t) D^2_{U_0},
\]

\[
\bar{h}_{i\eta_i}^{t-1} \leq \bar{h}_{i\eta_i}^t \leq \bar{h}_{i\eta_i}^{t-1} + (\eta_i^{t-1} - \eta_i^t) D^2_{U_i}, \ i = 1, \cdots, \bar{m}. \tag{A.1.20}
\]
The algorithm (see Algorithm 5) of solving the general structured nonsmooth problems (with \( \tilde{f} \) and \( \tilde{h} \) respectively approximated by \( \tilde{f}_{\eta_0} \) and \( \tilde{h}_{\eta_0} \)) is similar to Algorithm 2, except that the linear approximations of the objective function and constraint are replaced by \( \ell_{\tilde{f}_{\eta_0}}(x', x) := \tilde{f}_{\eta_0}(x') + \langle \nabla \tilde{f}_{\eta_0}(x'), x - x' \rangle \) and \( \ell_{\tilde{h}_{\eta_0}}(x', x) := \tilde{h}_{\eta_0}(x') + \langle \nabla \tilde{h}_{\eta_0}(x'), x - x' \rangle, i = 1, \cdots, \tilde{m} \), respectively. If the original functions are smooth, then the parameters \( \eta_i \) simply reduces to constant zero.

**Algorithm 5** CGO for Structured Nonsmooth Problems

The algorithm is modified from Algorithm 2 by replacing step (2.9) with

\[
\tilde{h}_t = \ell_{\tilde{h}_{\eta_{t-1}}}(x_{t-2}, p_{t-1}) + \lambda_t [\ell_{\tilde{h}_{\eta_{t-1}}}(x_{t-2}, p_{t-1}) - \ell_{\tilde{h}_{\eta_{t-2}}}(x_{t-3}, p_{t-2})], \tag{A.1.21}
\]

and primal update (2.12) with

\[
p_t = \arg\min_{x \in X} \ell_{\tilde{f}_{\eta_t}}(x_{t-1}, x) + (\ell_{\tilde{h}_{\eta_t}}(x_{t-1}, x), r_t), \tag{A.1.22}
\]

and update of lower bound functionals (2.14) and (2.15) with

\[
\tilde{f}_t(x) = (1 - \alpha_t) \tilde{f}_{t-1}(x) + \alpha_t \ell_{\tilde{f}_{\eta_t}}(x_{t-1}, x), \tag{A.1.23}
\]

\[
\tilde{h}_t(x) = (1 - \alpha_t) \tilde{h}_{t-1}(x) + \alpha_t (\ell_{\tilde{h}_{\eta_t}}(x_{t-1}, x), r_t). \tag{A.1.24}
\]

**A.1.3.1. Convergence Analysis** For the original nonsmooth problem, the gap function is defined by

\[
\tilde{Q}_t(w_t, w) := \tilde{f}(x_t) + \langle \tilde{h}(x_t), z \rangle - \tilde{f}(x) - \langle \tilde{h}_t(x), z_t \rangle, \forall w \in \tilde{X} \times \tilde{Z}.
\]

In view of Lemma 2.2, we can show that \( (\tilde{f}_t + \tilde{h}_t)(\cdot) \) computed from (A.1.23) and (A.1.24) is a lower bounding function of both the original objective \( \tilde{f}(x_t) + \langle \tilde{h}(x_t), z \rangle \) and the smoothing approximation \( \tilde{f}_{\eta_t}(x_t) + \langle \tilde{h}_{\eta_t}(x_t), z \rangle \). The gap function of the approximated problem is hereby defined as

\[
\tilde{Q}^\eta_t(w_t, w) := \tilde{f}_{\eta_t}(x_t) + \langle \tilde{h}_{\eta_t}(x_t), z \rangle - \tilde{f}(x) - \tilde{h}(x), \forall w \in \tilde{X} \times \tilde{Z}, \tag{A.1.25}
\]

for \( w_t := (x_t, z_t) \). Following from (A.1.18), it is easy to see that

\[
\tilde{Q}_t(w_t, w) \leq \tilde{Q}^\eta_t(w_t, w) + \eta^2_0 D_{U_0}^2 + \sum_{i=1}^{\tilde{m}} z_i \eta^2_i D^2_{U_i}, \quad k \geq 1, \forall w \in \tilde{X} \times \tilde{Z}. \tag{A.1.26}
\]
We will show in Theorem A.1.1 the iteration complexity of solving the nonsmooth problem is bounded by $O(1/\epsilon^2)$. To this end, we start by identifying an important recursion relation of the gap function (A.1.25) in Proposition A.1.3. Then in Proposition A.1.4, we state the convergence property under general parameter setup. In the subsequent analysis, we use the following notations:

\[ M_{B,U} := \sqrt{\sum_{i=1}^{m} M_{B,U}^2}, \quad L_h^i := (L_{h_1,n_1}, \ldots, L_{h_m,n_m}) \quad \text{and} \quad \bar{h}_{\eta'} := \left( \bar{h}_{1,n_1'}, \ldots, \bar{h}_{m,n_m'} \right). \]

**Proposition A.1.3.** At iteration $t > 1$, we have

\[
\tilde{Q}_t^n(w_t, w) \leq (1 - \alpha_t) \tilde{Q}_{t-1}^n(w_{t-1}, w) + \frac{(L_f^t + z^\top L_h^t) \alpha_t^2 D_x^2}{2} + (1 - \alpha_t) \left[ (\eta_0^{t-1} - \eta_0^{t}) D_{U_0}^2 + \sum_{i=1}^{m} z_i (\eta_i^{t-1} - \eta_i^{t}) D_{U_i}^2 \right] \]

\[ + \frac{6\alpha_t \lambda^2 M_{B,U}^2 D_x^2}{\tau_t} \quad \text{and} \quad \tilde{Q}_t^n(w_t, w) \leq (1 - \alpha_t) \left[ f_0^n(x_{t-1}) + (\bar{h}_{\eta'}(x_{t-1}), z) - f_{t-1}(x) - h_{t-1}(x) \right] + \frac{(L_f^t + z^\top L_h^t) \alpha_t^2 D_x^2}{2} \]

\[ + \frac{6\alpha_t \lambda^2 M_{B,U}^2 D_x^2}{\tau_t} \quad \text{and} \quad \tilde{Q}_t^n(w_t, w) \leq (1 - \alpha_t) \left[ f_0^n(x_{t-1}) + (\bar{h}_{\eta'}(x_{t-1}), z) - f_{t-1}(x) - h_{t-1}(x) \right] + \frac{(L_f^t + z^\top L_h^t) \alpha_t^2 D_x^2}{2} \]

\[ + \frac{6\alpha_t \lambda^2 M_{B,U}^2 D_x^2}{\tau_t}. \]

**Proof.** Using the relation in (A.1.20), the updates in (A.1.23), (A.1.24) and applying Lemma A.1.3 on $\bar{f}_0^n$, $\bar{h}_{\eta'}$, we have

\[
\tilde{Q}_t^n(w_t, w) \leq (1 - \alpha_t) \left[ f_0^n(x_{t-1}) + (\bar{h}_{\eta'}(x_{t-1}), z) - f_{t-1}(x) - h_{t-1}(x) \right] + \frac{(L_f^t + z^\top L_h^t) \alpha_t^2 D_x^2}{2} \]

\[ + \frac{6\alpha_t \lambda^2 M_{B,U}^2 D_x^2}{\tau_t}. \]

Note that the last line in (A.1.28) has the following relation:

\[
\ell_{f_0^n}(x_{t-1}, p_t) + (\ell_{\bar{h}_{\eta'}}(x_{t-1}, p_t), z) - \ell_{\bar{h}_{\eta'}}(x_{t-1}, x) - (\ell_{\bar{h}_{\eta'}}(x_{t-1}, x), r_t) \]

\[ \leq (\ell_{\bar{h}_{\eta'}}(x_{t-1}, p_t), z - r_t) \]

\[ \leq (\ell_{\bar{h}_{\eta'}}(x_{t-1}, p_t) - \bar{h}_{\eta'}(x_{t-1}, x) - r_t) + \tau_t V(r_{t-1}, z) - \tau_t V(r_t, z) - \tau_t V(r_{t-1}, r_t) \]

\[ = (\ell_{\bar{h}_{\eta'}}(x_{t-1}, p_t) - \ell_{\bar{h}_{\eta'}}(x_{t-2}, p_{t-1}), z - r_t) - \lambda_t \left( (\ell_{\bar{h}_{\eta'}}(x_{t-2}, p_{t-1}) - \ell_{\bar{h}_{\eta'}}(x_{t-3}, p_{t-2}), z - r_{t-1}) \right) \]

\[ + \tau_t V(r_{t-1}, z) - \tau_t V(r_t, z) \]

\[- \lambda_t \left( (\ell_{\bar{h}_{\eta'}}(x_{t-2}, p_{t-1}) - \ell_{\bar{h}_{\eta'}}(x_{t-3}, p_{t-2}), r_{t-1} - r_t) \right) - \tau_t V(r_{t-1}, r_t), \]

(A.1.29)
where the first inequality follows from the primal update in (A.1.22), the second inequality is the result of the dual update and Lemma A.1.1 and the last equality is by the definition of $\tilde{h}_i$ in (A.1.21).

Moreover, the last line in (A.1.29) can be bounded by

$$\begin{align*}
- \lambda_t & \left( \ell_{\tilde{h}_{i_t-1}}(x_{t-2}, p_{t-1}) - \ell_{\tilde{h}_{i_t-2}}(x_{t-3}, p_{t-2}, r_{t-1} - r_t) \right) - \tau_t V(r_{t-1}, r_t) \\
& \leq \frac{\alpha^2}{2\tau_t} \sum_{i=1}^{m} \left( \ell_{\tilde{h}_{i, \eta_t}}(x_{t-2}, p_{t-1}) - \ell_{\tilde{h}_{i, \eta_{t-1}}}(x_{t-3}, p_{t-2}) \right)^2 \\
& = \frac{\lambda^2}{2\tau_t} \sum_{i=1}^{m} \left( \tilde{h}_{i, \eta_{t-1}}(x_{t-2}) - \tilde{h}_{i, \eta_{t-2}}(x_{t-3}) + \langle \nabla \tilde{h}_{i, \eta_{t-1}}(x_{t-2}), p_{t-1} - x_{t-2} \rangle + \langle \nabla \tilde{h}_{i, \eta_{t-2}}(x_{t-3}), x_{t-3} - p_{t-2} \rangle \right)^2 \\
& \leq \frac{3\lambda^2}{2\tau_t} \sum_{i=1}^{m} \left[ \left( \tilde{h}_{i, \eta_{t-1}}(x_{t-2}) - \tilde{h}_{i, \eta_{t-2}}(x_{t-3}) \right)^2 + 2M_{B_i, U_i}^2 D_X^2 \right] \\
& \leq \frac{3\lambda^2}{2\tau_t} \sum_{i=1}^{m} \left[ 2 \left( \langle \nabla \tilde{h}_{i, \eta_{t-2}}(x_{t-3}), x_{t-3} - p_{t-2} \rangle \right)^2 + 2(\eta_{t-2}^i - \eta_{t-1}^i)^2 D_{U_i}^4 + 2M_{B_i, U_i}^2 D_X^2 \right] \\
& \leq \frac{6\alpha^2 M_{B_i, U_i}^2 D_X^2}{\tau_t} + \frac{3\lambda^2}{\tau_t} \sum_{i=1}^{m} (\eta_{t-2}^i - \eta_{t-1}^i)^2 D_{U_i}^4. \\
& \quad \text{(A.1.30)}
\end{align*}$$

The result of (A.1.27) follows from plugging relations (A.1.29) and (A.1.30) into (A.1.28).

**Proposition A.1.4.** Suppose that parameters $\alpha_t, \lambda_t, \tau_t$ in Algorithm 5 satisfy (A.1.12), the smoothing parameters $\eta_t^i$ satisfy the relation in (A.1.19). Then for any $T \geq 1$,

$$\begin{align*}
Q_T(w_T, w) & \leq \Gamma_T \sum_{t=1}^{T} \frac{\alpha_t}{\Gamma_t} \left[ \frac{\alpha_t \left( L_j + z^T L_h^t \right) D_X^2}{2} + \eta_0^2 D_{U_0}^2 + \sum_{i=1}^{m} z_i \eta_i^2 D_{U_i}^4 \right] \\
& \quad + \frac{6\lambda^2 M_{B_i, U_i}^2 D_X^2}{\tau_t} + \frac{3\lambda^2}{\tau_t} \sum_{i=1}^{m} (\eta_{t-2}^i - \eta_{t-1}^i)^2 D_{U_i}^4 \\
& \quad + \frac{6\alpha T \lambda^2 M_{B_i, U_i}^2 D_X^2}{\tau_T} + \frac{3\alpha T \lambda^2}{\tau_T} \sum_{i=1}^{m} (\eta_{t-1}^i - \eta_{t-1}^i)^2 D_{U_i}^4 + \alpha T \tau_T V \\\n& \quad + \eta_0^2 D_{U_0}^2 + \sum_{i=1}^{m} z_i \eta_i^T D_{U_i}^2, \\
& \forall w \in X \times Z.
\end{align*}$$

(A.1.31)
proof. Applying Lemma A.1.2 and Proposition A.1.3, we obtain

\[
Q_T^T(w_T, w) \leq \Gamma_T \sum_{t=1}^{T} \frac{\alpha_t}{\Gamma_t} \left[ \frac{\alpha_t \left( L_T^T + z^T L_h^T D_X^2 \right)}{2} + \frac{6\lambda_t^2 M_{B,U}^2 D_X^2}{\tau_t} + \frac{3\lambda_t^2}{\tau_t} \sum_{i=1}^{m} (\eta_t^{i,-2} - \eta_t^{i-1})^2 D_{U_i}^2 \right] \\
+ \frac{1 - \alpha_t}{\Gamma_t} \left[ \left( \eta_0^{i-1} - \eta_0^{i} \right) D_{U_0}^2 + \sum_{i=1}^{m} z_i (\eta_t^{i-1} - \eta_t^{i}) D_{U_i}^2 \right] \\
+ \Gamma_T \sum_{t=1}^{T} \frac{\alpha_t \tau_t}{\Gamma_t} \left[ \langle \ell_{h,t} (x_{t-1}, p_t) - \ell_{h,t-1} (x_{t-2}, p_{t-1}), z - r_t \rangle \\
- \lambda_t \langle \ell_{h,t-1} (x_{t-2}, p_{t-1}) - \ell_{h,t-2} (x_{t-3}, p_{t-2}), z - r_{t-1} \rangle \right] \\
+ \Gamma_T \sum_{t=1}^{T} \frac{\alpha_t \tau_t}{\Gamma_t} (V(r_{t-1}, z) - V(r_t, z)) \\
= \Gamma_T \sum_{t=1}^{T} \frac{\alpha_t}{\Gamma_t} \left[ \frac{\alpha_t \left( L_T^T + z^T L_h^T D_X^2 \right)}{2} + \eta_0^T D_{U_0}^2 + \sum_{i=1}^{m} z_i \eta_t^i D_{U_i}^2 \\
+ \frac{6\lambda_t^2 M_{B,U}^2 D_X^2}{\tau_t} + \frac{3\lambda_t^2}{\tau_t} \sum_{i=1}^{m} (\eta_t^{i,-2} - \eta_t^{i-1})^2 D_{U_i}^2 \right] \\
+ \Gamma_T \sum_{t=1}^{T} \frac{\alpha_t}{\Gamma_t} \left[ \langle \ell_{h,t} (x_{t-1}, p_t) - \ell_{h,t-1} (x_{t-2}, p_{t-1}), z - r_t \rangle \\
- \lambda_t \langle \ell_{h,t-1} (x_{t-2}, p_{t-1}) - \ell_{h,t-2} (x_{t-3}, p_{t-2}), z - r_{t-1} \rangle \right] \\
+ \Gamma_T \sum_{t=1}^{T} \frac{\alpha_t \tau_t}{\Gamma_t} (V(r_{t-1}, z) - V(r_t, z)), \tag{A.1.32}
\]

where the second equality follows from

\[
\sum_{t=1}^{T} \frac{1 - \alpha_t}{\Gamma_t} \left( (\eta_0^{i-1} - \eta_0^{i}) D_{U_0}^2 + \sum_{i=1}^{m} z_i (\eta_t^{i-1} - \eta_t^{i}) D_{U_i}^2 \right) = \sum_{t=1}^{T} \frac{\alpha_t}{\Gamma_t} \left( \eta_0^T D_{U_0}^2 + \sum_{i=1}^{m} z_i \eta_t^i D_{U_i}^2 \right).
\]

Similar to the derivation in (A.1.14), the last line in (A.1.32) follows

\[
\Gamma_T \sum_{t=1}^{T} \frac{\alpha_t \tau_t}{\Gamma_t} (V(r_{t-1}, z) - V(r_t, z)) \leq \alpha_T \tau_T \left( \bar{V} - V(r_T, z) \right). \tag{A.1.33}
\]
where the last inequality follows from Young’s inequality and the initialization condition \( x_0 = x_{-1} = x_{-2}, \ p_0 = p_{-1}. \)

Finally, by the inequality (A.1.26) with \( t = T \) and the results in (A.1.32), (A.1.33) and (A.1.34), we reach the conclusion in (A.1.31). □

Proposition A.1.4 can be easily extended to the convex constrained problem (2.1). More explicitly,

\[
Q_T(w_T, w) \leq \Gamma_T \sum_{t=1}^{T} \frac{\alpha_t}{\Gamma_t} \left[ \frac{\alpha_t z^T L^t_{i} D^2_{X}}{2} + z_i^T \eta_i D^2_{U_i} \right] + \frac{6\alpha_t^2 M^2_{B,U} D^2_{X}}{\tau_t} + 3\alpha_t^2 \frac{\sum_{i=0}^{m} (\eta_t^{i-2} - \eta_t^{i-1})^2 D^4_{U_i}}{\tau_t} + \frac{6\alpha_t \lambda^2_{i} M^2_{B,U} D^2_{X} \bar{\alpha}}{\tau_t} + \frac{3\alpha_t \lambda^2_{i} \sum_{i=0}^{m} (\eta_t^{i-2} - \eta_t^{i-1})^2 D^4_{U_i} + \alpha_t \tau_t V}{\tau_t} + \eta_T^T D^2_{U_0} + \sum_{i=0}^{m} z_i^T \eta_i^T D^2_{U_i}.
\]

and

\[
\|H(x_T, f^*)\|_\infty \leq \Gamma_T \sum_{t=1}^{T} \frac{\alpha_t}{\Gamma_t} \left[ \frac{\alpha_t \max_{i=1,\ldots,m} L^t_{i} D^2_{X}}{2} + \max_{i=1,\ldots,m} \eta_i^T D^2_{U_i} \right] + \frac{6\alpha_t^2 M^2_{B,U} D^2_{X}}{\tau_t} + 3\alpha_t^2 \frac{\sum_{i=0}^{m} (\eta_t^{i-2} - \eta_t^{i-1})^2 D^4_{U_i}}{\tau_t} + \frac{6\alpha_t \lambda^2_{i} M^2_{B,U} D^2_{X} \bar{\alpha}}{\tau_t} + \frac{3\alpha_t \lambda^2_{i} \sum_{i=0}^{m} (\eta_t^{i-2} - \eta_t^{i-1})^2 D^4_{U_i} + \alpha_t \tau_t V}{\tau_t} + \eta_T^T D^2_{U_0} + \max_{i=1,\ldots,m} \eta_i^T D^2_{U_i}.
\]

Theorem A.1.1 below demonstrates convergence rate of Algorithm 5.

**Theorem A.1.1.** Suppose parameters \( \alpha_t, \lambda_t \) and \( \tau_t \) are specified according to (2.22), with \( \bar{M} \) replaced \( M_{B,U} \) and

\[
\eta_t^i = \frac{\|B_iD_8^8\}}{\sqrt{T}U_i}, i = 0, 1, \cdots, m,
\]
then for $t \geq 1$, we have

$$Q_t(w_t, w) \leq \frac{8D_X \left( \|B_0\|D_U^0 + \sum_{i=1}^{\bar{m}} z_i \|B_i\|D_{U_i}^0 \right)}{3\sqrt{t+1}} + \frac{4D_X \sum_{i=1}^{\bar{m}} \|B_i\|^2D_{U_i}^0}{3M_{B,U}t(t+1)} + \frac{8M_{B,U}D_X}{9\sqrt{t+1}}$$

$$+ \frac{4\bar{M}_{B,U}D_X}{3(t+1)\sqrt{t}} + \frac{2D_X \sum_{i=1}^{\bar{m}} \|B_i\|^2D_{U_i}^0}{3\sqrt{t+1}} + \frac{18\bar{M}_{B,U}D_X \bar{V}}{\sqrt{t+1}} + \frac{D_X \left( \|B_0\|D_U^0 + \sum_{i=1}^{\bar{m}} z_i \|B_i\|D_{U_i} \right)}{\sqrt{t}}.$$  \hspace{0.5cm} (A.1.35)

**Proof.** Note first, since $\sqrt{t-1} \geq \sqrt{t-2}$, then

$$(\eta_t^{(2)} - \eta_t^{(1)})^2 = \frac{\|B_i\|^2D_{U_i}^0}{D_{U_i}} \left( \frac{1}{\sqrt{t-2}} - \frac{1}{\sqrt{t-1}} \right)^2 \leq \frac{\|B_i\|^2D_{U_i}^0}{D_{U_i}^2} \frac{1}{(t-1)(t-2)}.$$  

Therefore,

$$\sum_{t=3}^{T} \frac{3\alpha_t\lambda_t^2}{\Gamma_t\tau_t} \sum_{i=1}^{\bar{m}} (\eta_t^{(2)} - \eta_t^{(1)})^2 D_{U_i}^t \leq \frac{D_X}{3M_{B,U}} \sum_{i=1}^{\bar{m}} \|B_i\|^2D_{U_i}^0 \sum_{t=3}^{T} \frac{(t-1)^2}{\sqrt{tt(t-1)(t-2)}}$$

$$\leq \frac{2D_X}{3M_{B,U}} \sum_{i=1}^{\bar{m}} \|B_i\|^2D_{U_i}^0,$$  \hspace{0.5cm} (A.1.36)

where the last inequality follows from the relation

$$\sum_{t=3}^{T} \frac{(t-1)^2}{\sqrt{tt(t-1)(t-2)}} \leq \sum_{t=3}^{T} \frac{1}{(t-2)^{3/2}} \leq \int_{3}^{T} \frac{1}{(t-2)^{3/2}} \leq 2.$$  

Besides,

$$\sum_{t=1}^{T} \frac{\alpha_t}{\Gamma_t} \left( \eta_0^2D_{U_0}^2 + \sum_{i=1}^{\bar{m}} z_i \eta_i^2D_{U_i}^2 \right) = D_X \left( \|B_0\|D_U^0 + \sum_{i=1}^{\bar{m}} z_i \|B_i\|D_{U_i} \right) \sum_{t=1}^{T} \sqrt{t}$$

$$\leq \frac{2D_X \left( \|B_0\|D_U^0 + \sum_{i=1}^{\bar{m}} z_i \|B_i\|D_{U_i} \right)}{3} T\sqrt{T}.$$  \hspace{0.5cm} (A.1.37)
Moreover, since $\omega_i \geq 0$, $i = 0, 1, \ldots, \tilde{m}$, then $L_i = \frac{\|B_0\|^2}{\nu_0^{\omega_i + \nu_0}} \leq \frac{\|B_0\|^2}{\nu_0}$, $L_i = \frac{\|B_0\|^2}{\omega_i + \nu_0} \leq \frac{\|B_i\|^2}{\nu_0}$, $i = 1, \ldots, \tilde{m}$ and

$$\sum_{t=1}^T \frac{\zeta_t^2}{2t} (L_t^f + z_t^T L_t^f) D_X^2 \leq D_X \left(\|B_0\|D_{U_0} + \sum_{i=1}^{\tilde{m}} z_i \|B_i\|D_{U_i}\right) \sum_{t=1}^T \frac{\sqrt{t}}{t+1} \tag{A.1.38}$$

where the last inequality is due to $\sum_{t=1}^T \frac{\sqrt{t}}{t+1} \leq \frac{2}{\sqrt{T}}$.

Using the relations in (A.1.36), (A.1.37), (A.1.38), similar to (A.1.15), we can show that

$$\hat{Q}_t^p(w_t, w) \leq \frac{8D_X \left(\|B_0\|D_{U_0} + \sum_{i=1}^{\tilde{m}} z_i \|B_i\|D_{U_i}\right)}{3\sqrt{t+1}} + \frac{4D_X \sum_{i=1}^{\tilde{m}} \|B_i\|^2 D_{U_i}^2}{3M_{B,U}T(t+1)} + \frac{8M_{B,U}D_X}{9\sqrt{T+1}}$$

$$+ \frac{4M_{B,U}D_X}{3T(t+1)\sqrt{T}} + \frac{2D_X \sum_{i=1}^{\tilde{m}} \|B_i\|^2 D_{U_i}^2}{3T^2(t+1)\sqrt{T}M_{B,U}} + \frac{18M_{B,U}D_X V}{\sqrt{T+1}}.$$

We conclude the result in (A.1.35) by noting that $\eta_0^T D_{U_0}^2 + \sum_{i=0}^{\tilde{m}} z_i \eta_i^T D_{U_i}^2 \leq \frac{D_X \|B_0\|D_{U_0}}{\sqrt{T}} + \frac{D_X \sum_{i=1}^{\tilde{m}} z_i \|B_i\|D_{U_i}}{\sqrt{T}}$.

Similarly, for problem (2.1) with structured nonsmooth functions, we conclude that

$$Q_t(w_t, w) \leq \frac{8D_X \left(\sum_{i=0}^{m+1} z_i \|B_i\|D_{U_i}\right)}{3\sqrt{t+1}} + \frac{4D_X \sum_{i=0}^{m+1} \|B_i\|^2 D_{U_i}^2}{3M_{B,U}t(t+1)} + \frac{8M_{B,U}D_X}{9\sqrt{T+1}}$$

$$+ \frac{4M_{B,U}D_X}{3(t+1)\sqrt{t}} + \frac{2D_X \sum_{i=0}^{m+1} \|B_i\|^2 D_{U_i}^2}{3t^2(t+1)\sqrt{t}M_{B,U}} + \frac{18M_{B,U}D_X V}{\sqrt{t+1}} + \frac{D_X \sum_{i=0}^{m+1} z_i \|B_i\|D_{U_i}}{\sqrt{t}}.$$

$$\|H(x_T, f^*)\|_{\infty} \leq \frac{8D_X \left(\sum_{i=0}^{m+1} \|B_i\|D_{U_i}\right)}{3\sqrt{t+1}} + \frac{4D_X \sum_{i=0}^{m+1} \|B_i\|^2 D_{U_i}^2}{3M_{B,U}t(t+1)} + \frac{8M_{B,U}D_X}{9\sqrt{T+1}}$$

$$+ \frac{4M_{B,U}D_X}{3(t+1)\sqrt{t}} + \frac{2D_X \sum_{i=0}^{m+1} \|B_i\|^2 D_{U_i}^2}{3t^2(t+1)\sqrt{t}M_{B,U}} + \frac{18M_{B,U}D_X V}{\sqrt{t+1}} + \frac{D_X \sum_{i=0}^{\max(m+1)} \|B_i\|D_{U_i}}{\sqrt{t}}.$$

### A.2. Convergence Analysis of LCG

**Lemma 2.1** At iteration $k$, if Algorithm 1 does not terminate, then $L_k > 0$. Moreover, the sequence of the level estimates satisfies $l_1 < \cdots < l_k < l_{k+1} < \cdots \leq f^*$, $k \geq 1$. Consequently, $\phi(l_{k+1}) \geq \phi(l_k) \geq \cdots \geq \phi(f^*) = 0$. 


Proof. We first show that at iteration \( k \), if the algorithm does not terminate, then \( L_k > 0 \). Indeed, if, on the opposite, \( L_k \leq 0 \), since CGO stops at \( U_k - L_k \leq (1 - \mu) \epsilon \), then \( U_k \leq (1 - \mu) \epsilon + L_k \leq (1 - \mu) \epsilon \leq \epsilon \), leading to the termination of the algorithm. Therefore, together by the requirement that \( \gamma_k > 0 \) returned by CGO, at each update of \( l \), we have \( l_{k+1} - l_k \geq \frac{1}{\gamma_k} \epsilon > 0 \). In addition, noting that \( L_k(l_{k+1}) = 0 \) by the origin of \( l_{k+1} \) in (2.3), and that \( \phi(l_{k+1}) \geq L_k(l_{k+1}) \) since \( L \) underestimates \( \phi \), we have \( \phi(l_{k+1}) \geq L_k(l_{k+1}) = 0 = \phi(f^*) \), which, in view of the fact that \( \phi \) is nonincreasing, implies that \( l_{k+1} \leq f^*, k \geq 1 \). By the definition of \( l_1 \), we have \( l_1 \leq f^* \). Finally by the monotonicity non-increasing property of \( \phi \) and \( \phi(f^*) \), we have \( \phi(l_{k+1}) \geq \phi(l_k) \geq \cdots \geq \phi(f^*) = 0 \). \( \square \)

**Theorem 2.1** For all \( k \geq 1 \), we have

\[
U_k \leq (f^* - l_1) \frac{1}{\mu} \left( \frac{1}{2 \mu} \right)^k,
\]

where \( \mu \in (\frac{1}{2}, 1) \), \( l_1 \) is the initial estimate of the optimal value of (1.1) such that \( l_1 \leq f^* \). Moreover, given precision \( \epsilon \), at the termination of LCG when \( U_k \leq \epsilon \), the algorithm yields an \( \epsilon \)-optimal and \( \epsilon \)-feasible solution \( x_k \) of problem (1.1).

Proof. By the linearity of \( L_k(\cdot) \) and the relation that \( l_{k-1} < l_k < l_{k+1} \) according to Lemma 2.1, we have

\[
\frac{L_k(l_{k-1}) - L_k(l_k)}{l_k - l_{k-1}} = \frac{L_k(l_k) - L_k(l_{k+1})}{l_{k+1} - l_k},
\]

which together with the fact \( L_k(l_{k+1}) = 0 \) and the simple relation \( a + b \geq 2 \sqrt{ab}, \ a, b \in \mathbb{R}^+ \) imply that

\[
(l_{k+1} - l_k) L_k(l_{k-1}) \geq (l_{k+1} - l_k + l_k - l_{k-1}) L_k(l_k) = 2 \sqrt{l_{k+1} - l_k} \sqrt{l_k - l_{k-1}} L_k(l_k).
\]

Rearranging the terms, we obtain

\[
\frac{L_k(l_{k-1})}{\sqrt{l_k - l_{k-1}}} \geq \frac{2 L_k(l_k)}{\sqrt{l_{k+1} - l_k}}. \quad (A.2.2)
\]

Observe that \( U_k - L_k \leq (1 - \mu) \epsilon \) and \( U_k > \epsilon \) when the algorithm does not terminate at iteration \( k \). Therefore, we have \( U_k - L_k \leq (1 - \mu) U_k \), and thus \( L_k / U_k \geq \mu \). Using this observation and the fact \( L_k(l_k) = L_k \), we obtain \( L_k(l_k) \geq \mu U_k \). Note also \( U_{k-1} \geq \phi(l_{k-1}) \geq L_k(l_{k-1}) \). Using this bound and the one in (A.2.2), we have

\[
\frac{U_{k-1}}{\sqrt{l_k - l_{k-1}}} \geq \frac{2 \mu U_k}{\sqrt{l_{k+1} - l_k}}. \quad (A.2.3)
\]
Applying the above relation recursively and the facts that \( U_1 \leq \frac{1}{\mu} L_1, L_1 \leq \phi(l_1), l_{k+1} - l_k \leq f^* - l_1 \) yields

\[
U_k \leq \frac{1}{2\mu} \left( \frac{l_{k+1} - l_k}{l_k - l_{k-1}} U_{k-1} \right) \\
\leq \left( \frac{1}{2\mu} \right)^{k-1} \left( \frac{l_{k+1} - l_k}{l_2 - l_1} \right) U_1 \\
\leq \frac{1}{\mu} \left( \frac{1}{2\mu} \right)^{k-1} \sqrt{(f^* - l_1)\phi(l_1)} \sqrt{\frac{L_1}{l_2 - l_1}}.
\]

(A.2.4)

Note also it can be easily verified that: \( \phi(l) - \phi(l + \delta) \leq \delta, \ l \in \mathbb{R} \), for any \( \delta \geq 0 \) (same for \( \mathcal{L}_1(\cdot) \)), which leads to \( \phi(l_1) \leq f^* - l_1 \) and \( \mathcal{L}_1(l_1) \leq l_2 - l_1 \) as \( \mathcal{L}_1(l_2) = 0 \) and \( \phi(f^*) = 0 \). Consequently, following from the relation in (A.2.4), we attain

\[
U_k \leq \frac{1}{\mu} \left( \frac{1}{2\mu} \right)^{k-1} (f^* - l_1).
\]

At the termination of LCG when \( U_k \leq \epsilon \), the algorithm yields an \( \epsilon \)-optimal and \( \epsilon \)-feasible solution \( x_k \) of problem (1.1) since \( f(x_k) - f^* \leq f(x_k) - l_k \leq U_k \leq \epsilon \) and \( \max_{i=1,\ldots,m} \{ h_i(x_k) \} \leq U_k \leq \epsilon \). □

**Lemma 2.3** When LCG does not terminate at iteration \( k \), the output \((\gamma_k, L_k, U_k)\) of CGO satisfies (2.4)-(2.6).

**Proof.** First define the sequence \( \{\beta^t\} \), across inner iteration (CGO iteration) \( t \geq 1 \) as follow:

\( \beta^t := (\beta^t_1, \ldots, \beta^t_t) \), where \( \beta^t_j := \begin{cases} \alpha_t, & \text{if } j = t, \\ (1 - \alpha_t) \beta^{t-1}_j, & \text{if } j \neq t, \end{cases} \) with \( \beta^1_1 = \alpha_1 \). Denote \( r_j := (r_{j,0}, \ldots, r_{j,m}) \), where \( r_{j,i} \) is the \( i \)-th element of vector \( r_j \) at iteration \( j, j \leq t \). According to Algorithm 2, \( \overline{h}_t(x; l) \) can be explicitly written as:

\[
\overline{h}_t(x; l) = -\gamma_t l + \sum_{j=1}^t \beta^t_j r_{j,0} l f(x_{j-1}, x) + \sum_{i=1}^m r_{j,i} l h_i(x_{j-1}, x),
\]

(A.2.5)

where \( \gamma_t = \sum_{j=1}^t \beta^t_j r_{j,0} \) and we have \( z_{t,i} = \sum_{j=1}^t \beta^t_j r_{j,i} \), \( z_{t,i} \) is the \( i \)-th element of vector \( z_t \) at iteration \( t \).

At each CGO iteration under outer iteration \( k \), by the definition in (2.2), we have \( \mathcal{L}_t(l) = L_t - \gamma_t (l - l_k) \). Arranging the terms and using the relation in (2.16) and (A.2.5), for each \( l \in \mathbb{R} \), we have

\[
\mathcal{L}_t(l) = -\gamma_t l + (L_t + \gamma_t l_k) \\
= -\gamma_t l + \min_{x \in X} \overline{h}_t(x; l_k) + \gamma_t l_k \\
= \min_{x \in X} \overline{h}_t(x; l).
\]

Moreover, according to Lemma 2.2, it can be shown that \( \overline{h}_t(x; l) \leq \gamma_t [f(x) - l] + \langle h(x), z_i \rangle, \forall x \in X \).

Hence, \( \mathcal{L}_t(l) = \min_{x \in X} \overline{h}_t(x; l) \leq \min_{x \in X} \gamma_t [f(x) - l] + \langle h(x), z_i \rangle \leq \min_{x \in X} \gamma [f(x) - l] + \langle h(x), z \rangle = \phi(l) \).
Immediately, we obtain the relation in (2.6). In view of Lemma 2.2 and the relation in (2.6), for a given level estimate \( l \in \mathbb{R} \), \( L_k, U_k \) are the lower bound and upper bound of \( \phi(l) \), respectively. Therefore, (2.5) is satisfied.

Now, we show (2.4). By (A.2.5), we have

\[
\mathcal{L}_t(l) = -\gamma_t l + \min_{x \in X} \sum_{j=1}^{t} \beta_j^2 \left[ r_j, \ell_j f(x_{j-1}, x) + \sum_{i=1}^{m} r_{j,i} \ell_{h_i}(x_{j-1}, x) \right].
\]

In the case where LCG is not terminated at outer iteration \( k \), suppose CGO runs \( t(k) \) iterations. According to Lemma 2.1, it produces a lower bound such that \( L_{t(k)} > 0 \). Here \( \gamma_k \equiv \gamma_{t(k)}, z_k \equiv z_{t(k)}, L_k \equiv L_{t(k)} \) and \( \mathcal{L}_k(l_k) \equiv \mathcal{L}_{t(k)}(l_k) \). If \( \gamma_k = 0 \), recall that \( \gamma_k = \sum_{j=1}^{t(k)} \beta_j^2 r_{j,0} \), then we must have \( r_{j,0} = 0 \), \( \forall j \leq t(k) \). This implies that \( L_k = L_k(l_k) = \min_{x \in X} \sum_{j=1}^{t(k)} \beta_j^2 \left( \sum_{i=1}^{m} r_{j,i} \ell_{h_i}(x_{j-1}, x) \right) = \min_{x \in X} \langle z_k, h(x) \rangle \leq 0 \), which leads to contradiction. This shows that CGO returns \( \gamma_k \) such that \( \gamma_k > 0 \). \( \Box \)

**Corollary A.2.1.** Suppose the algorithmic parameters of CGO are set to (2.22). Then for any \( t \geq 1 \) and \( \forall w \in (X, Z) \),

\[
Q_t(w_t, w) \leq \frac{2z^T L \bar{D}_{X}^2}{t + 1} + \frac{MD_X}{\sqrt{t + 1}} \left[ 18 \bar{V} + \frac{7}{6} \right],
\]

\[
f(x_t) - f^* \leq \frac{2 \max_{i=1, \ldots, m+1} L_{h_i} \bar{D}_{X}^2}{t + 1} + \frac{MD_X}{\sqrt{t + 1}} \left[ 18 \bar{V} + \frac{7}{6} \right],
\]

\[
\|h(x_t)\|_{\infty} \leq \frac{2 \max_{i=1, \ldots, m+1} L_{h_i} \bar{D}_{X}^2}{t + 1} + \frac{MD_X}{\sqrt{t + 1}} \left[ 18 \bar{V} + \frac{7}{6} \right].
\]

**Proof.** The convergence analysis on the gap function \( Q_t(w_t, w) \) is similar to the one on the general case when treating \( \bar{f}(\cdot) = 0 \) (see Theorem 2.2). We conclude that

\[
Q_t(w_t, w) \leq \frac{2z^T L \bar{D}_{X}^2}{t + 1} + \frac{MD_X}{\sqrt{t + 1}} \left[ 18 \bar{V} + \frac{7}{6} \right], \forall w := (x, z) \in X \times Z.
\]

Now we analyze the bound of \( \|h(x_t; f^*)\|_{\infty} \), thus the bounds of \( f(x_t) - f^* \) and of \( \|h(x_t)\|_{\ast} \). Suppose there exists at least one element of \( \bar{h}(x_t; f^*) \) is positive, otherwise, we arrive trivially at \( \|h(x_t; f^*)\|_{\ast} \leq 0 \). Define \( w' := (x^*, z') \), where \( x^* \) is the optimal primal solution. \( z' \) is defined as follows: \( z' \in Z, z'_j = 1 \) if \( j \) is one of the indices such that \( j \in \text{argmax}_{i=1, \ldots, m} \bar{h}_i(x_t; f^*) \) and \( z'_i = 0 \) otherwise. By the definition of \( z' \) and the relation \( h_j(x^*; f^*) \leq \langle \bar{h}(x^*; f^*), z_i \rangle \leq 0 \), we have

\[
Q_t(w_t, w') = \langle \bar{h}(x_t; f^*), z' \rangle - h_j(x^*; f^*) \geq \|h(x_t; f^*)\|_{\infty}.
\]
Note also,
\[ \|\tilde{h}(x_i; f^*)\|_\infty = \max \{ f(x_i) - f^*, h(x_i) \} \]
Then we have \( \forall w \in (X, Z) \),
\[ f(x_i) - f^* \leq \frac{2 \max_{i=1, \ldots, m+1} L_{h_i} D_X^2}{t+1} + \frac{MD_X}{\sqrt{t+1}} \left[ 18V + \frac{7}{6} \right], \]
\[ \|h(x_i)\|_\infty \leq \frac{2 \max_{i=1, \ldots, m+1} L_{h_i} D_X^2}{t+1} + \frac{MD_X}{\sqrt{t+1}} \left[ 18V + \frac{7}{6} \right]. \]

\[ \square \]

**Theorem 2.3** Suppose that the algorithmic parameters of CGO are set to (2.22). Then the total number of CGO iterations required to find an \( \epsilon \)-solution \( \bar{x} \in X \) of (1.1) can be bounded by \( \mathcal{O} \left( \frac{1}{\epsilon^2} \log \left( \frac{1}{\epsilon} \right) \right) \).

**Proof.** Using the result in Corollary A.2.1 and the fact that \( U_t - L_t = \max_{w \in X \times Z} Q_t(w_t, w) \), we immediately obtain
\[ U_t - L_t \leq \frac{2 \max_{i=1, \ldots, m+1} L_{h_i} D_X^2}{t+1} + \frac{MD_X}{\sqrt{t+1}} \left[ 18V + \frac{7}{6} \right]. \]
Consequently, given precision \( \epsilon > 0 \), to attain \( U_k - L_k \leq \epsilon \) at each call of CGO, the number of iterations is bounded by \( \mathcal{O} \left( \frac{1}{\epsilon^2} \right) \). Furthermore, in view of Theorem 2.1, the required number of outer loop iterations to obtain \( U_k \leq \epsilon \) and thus \( f(x_k) - f^* \leq \epsilon, \|h(x_k)\|_\infty \leq \epsilon \) is bounded by \( \mathcal{O} \left( \log \frac{1}{\epsilon} \right) \). Combining these two results, the overall iteration complexity of LCG solving the convex constrained problem (1.1) is \( \mathcal{O} \left( \frac{1}{\epsilon^2} \log \left( \frac{1}{\epsilon} \right) \right) \). \( \square \)

**A.3. Modified Level Conditional Gradient Method**

In this section, we focus on the modified version of LCG (MLCG), which generates a sequence of decreasing level estimates that approximate from above the optimal value of the problem. More specifically, we present the algorithmic framework of the MLCG method and convergence analysis of the outer loop. Remarkably, CGO requires no change in MLCG and remains as what it is in LCG.

To approximate the optimal value \( f^* \) by a sequence of decreasing level estimate from above, the original LCG (Algorithm 1, Section 2) mainly takes changes in the following steps: (1) In the initialization step, \( l_1 \) is required to overestimate \( f^* \). One plausible option is letting \( l_1 = f(x_0), \) s.t. \( x_0 \in X, h_i(x_0) \leq 0, i = 1, \ldots, m; \) (2) The update rule of the level estimate is changed to \( l_{k+1} = l_k + U_k; \) (3) The algorithm terminal condition is changed to \( L_k \geq -\epsilon \kappa. \) Here \( \kappa \) is a lower approximation of the condition number \( \kappa, \) where
\[ \kappa := \frac{\phi(l_1)}{l_1 - f^*}. \]
It can be easily verified that \( \kappa \leq 1 \). We can choose \( \tilde{\kappa} = -\frac{U_1}{l_1 - f} \), where \( \tilde{f} := \min\{f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle : x \in X \} \). In this way, \( \tilde{f} \leq f^* \) and \( \tilde{\kappa} \leq \kappa \). Similar to (Lin et al. 2018), the outer loop iteration complexity relies on \( \kappa \) and we will demonstrate later how the terminal condition \( L_k \geq -\epsilon \tilde{\kappa} \) implies the convergence of the outer loop. The MLCG method is summarized in Algorithm 6.

Algorithm 6 Modified Level Conditional Gradient Method (MLCG)

1: Inputs: \( \epsilon > 0, \mu \in (0, 1) \).
2: Initialization: \( x_0 \in X, h_i(x_0) \leq 0, i = 1, \ldots, m, l_1 = f(x_0) \).
3: for \( k = 1, 2, \ldots \) do
4: Call CGO with input \( l_k \) and obtain approximate solutions \( (x_k; (\gamma_k, z_k)) \in X \times Z \), lower bound \( L_k \), upper bound \( U_k \) and if \( k = 1 \), obtain \( \tilde{\kappa} = -\frac{U_1}{l_1 - f} \) such that \( U_k - L_k \leq (1 - \mu)\tilde{\kappa} \epsilon \).
5: if \( L_k \geq -\epsilon \tilde{\kappa} \) then
6: Terminate and return \( x_k \).
7: end if
8: \( l_{k+1} = l_k + U_k \).
9: end for

Remark A.3.1. There is one edge case such that \( l_1 = f^* \) leading to termination of the algorithm at iteration \( k = 1 \), thus we will not consider this situation in the convergence analysis. In this case, \( U_1 \geq \phi(l_1) = \phi(f^*) = 0 \). Let \( \tilde{\kappa} = \epsilon \) (instead of \( -\frac{U_1}{l_1 - f} \)). In view of CGO terminal condition, we have \( L_1 \geq U_1 - (1 - \mu)\tilde{\kappa} \epsilon \geq -(1 - \mu)\tilde{\kappa} \epsilon \geq -\tilde{\kappa} \epsilon \) and the algorithm terminates. Since \( l_1 = f^* \), the condition number \( \kappa \) does not exist. In fact, the algorithm terminates at \( k = 1 \), thus the iteration complexity in this case will not be affected by \( \kappa \).

A.3.1. Outer Loop Iteration Complexity of MLCG

We start with several lemmas that are of important use in the outer loop convergence analysis.

Lemma A.3.1. When MLCG is not terminated at iteration \( k \) \( (k \geq 1) \), then \( U_k \leq \mu L_k \).

Proof. We first demonstrate that \( U_k \geq 0 \) then the algorithm terminates at iteration \( k \). Indeed, at \( k > 1 \), if \( U_k \geq 0 \), then by the stopping criteria of CGO, \( L_k \geq U_k - (1 - \mu)\tilde{\kappa} \epsilon \geq -(1 - \mu)\tilde{\kappa} \epsilon \geq -\tilde{\kappa} \epsilon \).
Consequently, the algorithm terminates. At iteration \( k \), since the algorithm is not terminated, then \( L_k < -\epsilon \tilde{\kappa} \). By the stopping criteria of CGO such as \( U_k - L_k \leq (1 - \mu)\tilde{\kappa} \epsilon \), we have \( U_k - L_k \leq (1 - \mu)\tilde{\kappa} (L_k/\tilde{\kappa}) = (1 - \mu)(-L_k) \). Rearranging the terms in the above inequality, we arrive at \( U_k \leq \mu L_k \). \( \square \)

Lemma A.3.2. \( l_1 > \cdots > l_k > \cdots \geq f^* \).
Proof. We have discussed the case when \( l_1 = f^* \) in Remark A.3.1. We will focus on the case where \( l_1 > f^* \). We show \( l_{k+1} - f^* \geq 0 \) by induction. Suppose \( l_k - f^* \geq 0 \), then
\[
\begin{align*}
l_{k+1} - f^* & = l_k + U_k - f^* \\
& \geq l_k + \phi(l_k) - f^* \\
& \geq l_k - f^* - (l_k - f^*) \\
& = 0.
\end{align*}
\]
where the last inequality is due to \( \phi(f^*) - \phi(l_k) \leq l_k - f^* \) with \( l_k - f^* \geq 0 \) (induction assumption) and \( \phi(f^*) = 0 \). Next, we show that \( l_{k+1} < l_k \). By Lemma A.3.1, we have \( U_k \leq \mu L_k < 0 \) when the algorithm does not terminate, then \( l_{k+1} - l_k = U_k < 0 \).

The theorem below shows the outer iteration complexity of MLCG and demonstrates that when it terminates it outputs an \( \epsilon \)-optimal and \( \epsilon \)-feasible solution.

**Theorem A.3.1.** For \( k \geq 1 \), Algorithm 6 generates \( l_k \) that satisfies
\[
l_k - f^* \leq (1 - \kappa \mu)^{k-1} (l_1 - f^*),
\]
where \( \mu \in (0, 1), \kappa \in (0, 1] \) and \( l_1 \) is the initial level estimate of \( f^* \) such that \( l_1 > f^* \). Moreover, at the termination of Algorithm 6, it returns an \( \epsilon \)-optimal and \( \epsilon \)-feasible solution.

**Proof.** We have the following relation
\[
\begin{align*}
l_{k+1} - f^* & = l_k + U_k - f^* \\
& \leq l_k - f^* + \mu L_k \\
& \leq l_k - f^* + \mu \phi(l_k) \\
& \leq l_k - f^* - \mu \kappa (l_k - f^*) \\
& = (1 - \mu \kappa) (l_k - f^*).
\end{align*}
\]
The first inequality follows from Lemma A.3.1, the second inequality from \( L_k \leq \phi(l_k) \), the third is due to \( \frac{\phi(l_k) - \phi(f^*)}{l_k - f^*} \leq \frac{\phi(l_1) - \phi(f^*)}{l_1 - f^*} \equiv -\kappa \), which holds because of the convexity of \( \phi(\cdot) \) and the relation that \( l_k \leq l_1, k \geq 1 \). Using induction on \( k \), we have \( l_{k+1} - f^* \leq (1 - \kappa \mu)^k (l_1 - f^*) \).

Next, we will show that given precision \( \epsilon \), the terminal condition \( L_k \geq -\epsilon \bar{k} \) implies \( l_k - f^* \leq \epsilon \). Note first \( -\phi(l_k) \leq -L_k \) and \( -\phi(l_k) \geq \kappa (l_k - f^*) \). Using these inequalities and the relation that \( \bar{k} \leq \kappa \), we obtain \( l_k - f^* \leq -L_k / \kappa \leq \frac{\epsilon}{\kappa} \leq \epsilon \). Moreover, in view of Lemma A.3.2, we have \( L_k \leq \phi(l_k) \leq \phi(f^*) = 0 \), then \( U_k \leq L_k + (1 - \mu) \bar{k} \epsilon \leq (1 - \mu) \bar{k} \epsilon \). This implies that \( f(x_k) - f^* \leq (f(x_k) - l_k) + (l_k - f^*) \leq U_k + \frac{\epsilon}{\kappa} \leq \left( (1 - \mu) \bar{k} + \frac{\epsilon}{\kappa} \right) \epsilon \) and \( \max_{i=1, \ldots, m} h_i(x_k) \leq U_k \leq (1 - \mu) \bar{k} \epsilon \leq \epsilon \). \( \square \)
A.4. Convergence Analysis of Nonconvex Conditional Gradient Method

A.4.1. IPP-LCG for Nonconvex Problem

The following two lemmas serve as building blocks for establishing the convergence rate of IPP-LCG. In particular, Lemma A.4.1 characterizes an important property of the optimal solution of the subproblem (3.2) and Lemma A.4.2 states that the Slater condition enforces uniform boundness on \( y_j^* \).

**Lemma A.4.1.** If \( x_j^* \) is a KKT point (paired with \( y_j^* \)) of the subproblem (3.2), then \( \forall x \in X \),

\[
    f(x; x_{j-1}) - f(x_j^*; x_{j-1}) + \langle y_j^*, h(x) \rangle \geq \frac{L_f}{2} \| x_j^* - x \|^2.
\]

**Proof.** By (3.1), we have that \( f(\cdot; x') \) is strongly convex. Together by the strong convexity of \( f(\cdot; x_{j-1}) \) and convexity of \( h_i(\cdot) \) as well as the fact that \( y_j^* \geq 0 \), we have

\[
    f(x; x_{j-1}) + \langle y_j^*, h(x) \rangle \geq f(x_j^*; x_{j-1}) + \langle \nabla f(x_j^*; x_{j-1}), x - x_j^* \rangle + \frac{L_f}{2} \| x - x_j^* \|^2 + \sum_{i=1}^m y_{j,i}^* (h_i(x_j^*) + \langle \nabla h_i(x_j^*), x - x_j^* \rangle)
\]

\[
\geq f(x_j^*; x_{j-1}) + \frac{L_f}{2} \| x - x_j^* \|^2, \quad \forall x \in X,
\]

where the last inequality follows from properties of the KKT point that \( \sum_{i=1}^m y_{j,i}^* h_i(x_j^*) = 0 \) and \( \nabla f(x_j^*; x_{j-1}) + \sum_{i=1}^m y_{j,i}^* \nabla h_i(x_j^*) \) belongs to the normal cone of \( X \).

**Lemma A.4.2.** Suppose there exists \( \tilde{x} \in X \) such that \( h_i(\tilde{x}) < 0 \), \( i = 1, \ldots, m \), then the dual solution \( y_j^* \) is uniformly bounded such that

\[
\| y_j^* \|_1 \leq \frac{f(\tilde{x}) - f^* + L_f \| \tilde{x} \|_\infty}{\| h(\tilde{x}) \|_\infty},
\]

where \( \| \cdot \|_1 \) denote the \( \ell_1 \) norm and \( \| \tilde{x} \|_\infty = \max_{x,y \in X} \frac{1}{2} \| x - y \|^2 \).

**Proof.** Using Lemma A.4.1 and replacing \( x \) with \( \tilde{x} \), we have

\[
    -\langle y_j^*, h(\tilde{x}) \rangle \leq f(\tilde{x}; x_{j-1}) - f(x_j^*; x_{j-1}) - \frac{L_f}{2} \| \tilde{x} - x_j^* \|^2
    = f(\tilde{x}) - f(x_j^*) + L_f \left[ \| \tilde{x} - x_{j-1} \|^2 - \| x_j^* - x_{j-1} \|^2 \right] - \frac{L_f}{2} \| \tilde{x} - x_j^* \|^2
\]

\[
\leq f(\tilde{x}) - f(x_j^*) + \frac{L_f}{2} \| \tilde{x} - x_{j-1} \|^2
\]

\[
\leq f(\tilde{x}) - f(x_j^*) + \frac{L_f}{2} \| \tilde{x} - x_{j-1} \|^2 + L_f \| \tilde{x} \|_\infty.
\]

Note that \( h_i(\tilde{x}) \leq -\| h(\tilde{x}) \|_\infty, i = 1, \ldots, m \), then \( -\langle y_j^*, h(\tilde{x}) \rangle \geq \| y_j^* \|_1 \| h(\tilde{x}) \|_\infty \).
Theorem 3.1 The total number of CGO iterations performed by the IPP-LCG method to compute an \((\epsilon, \epsilon)\)-KKT point of problem (1.1) is bounded by \(O\left(\frac{1}{\epsilon^2} \log(\frac{1}{\epsilon})\right)\).

Proof. From Algorithm 3, we have \(\delta^j \geq f(x_j; x_{j-1}) - f(x_j^*; x_{j-1})\) and \(\delta^h \geq \|h(x_j)\|_\infty\). Define \(B := \frac{f(x) - f^* + L_f \overline{y}}{\|h(x)\|_\infty}\), \(\epsilon_f := \frac{2}{L_f} (\delta^f + B \delta^h)\), \(\epsilon'_j := \frac{8L_f}{J} [f(x_0) - f(x_j)] + \delta^f + B \delta^h\). Note first, since \((x_j^*, y_j^*)\) is a pair of optimal solution of subproblem (3.2), then the complementary slackness condition in (3.1) automatically holds, i.e. \(\sum_{i=1}^{m} [y_j^*_i, h_i(x_j^*)] = 0\), where \(y_j^*_i\) is the \(i\)-th element of \(y_j^*\).

By Lemma A.4.1 (replace \(x\) with \(x_j\)), we have
\[
\|x_j^* - x_j\|^2 \leq \frac{2}{L_f} \left[ f(x_j; x_{j-1}) - f(x_j^*; x_{j-1}) + \langle y_j^*, h(x_j) \rangle \right] \leq \frac{2}{L_f} (\delta^f + B \delta^h).
\]
Replacing \(x\) with \(x_{j-1}\) in Lemma A.4.1 and using the relations that \(f(x_j; x_{j-1}) - f(x_j^*; x_{j-1}) \leq \delta^f\) as well as \(h(x_j) \leq \delta^h\), we obtain
\[
\frac{L_f}{2} \|x_j^* - x_{j-1}\|^2 \leq f(x_{j-1}) - f(x_j^*; x_{j-1}) + \langle y_j^*, h(x_{j-1}) \rangle = f(x_{j-1}) - f(x_j) - L_f \|x_j - x_{j-1}\|^2 + \delta^f + B \delta^h \leq f(x_{j-1}) - f(x_j) + \delta^f + B \delta^h \leq \frac{1}{J} \sum_{j=1}^{J} f(x_{j-1}) - f(x_j) + \delta^f + B \delta^h \leq \frac{1}{J} [f(x_0) - f(x_j)] + \delta^f + B \delta^h,
\]
where the third inequality follows from the selection of \(\hat{j}\) in Algorithm 3. Using the above equality, and the KKT condition applied for (3.2), we arrive at
\[
\left[ d \left( \nabla f(x_j^*) + \sum_{i=1}^{m} y_j^* i \nabla h_i(x_j^*), -N_X(x_j^*) \right) \right]^2 = 4L_f^2 \|x_j^* - x_{j-1}\|^2 \leq \frac{8L_f}{J} [f(x_0) - f(x_j)] + \delta^f + B \delta^h.
\]
Combining (A.4.4) and (A.4.6), we reach the conclusion that \(x_j\) is an \((\epsilon'_j, \epsilon_j)\)-KKT point of problem (1.1). Consequently, given precision \(\epsilon\), combining the result in Theorem 2.3, the overall iteration complexity of IPP-LCG solving for an \((\epsilon, \epsilon)\)-KKT point is bounded by \(O\left(\frac{1}{\epsilon^2} \log(\frac{1}{\epsilon})\right)\). \(\Box\)

A.4.2. DNCG for Nonconvex Problem

Lemma 3.1 \(\tilde{F}(\cdot)\) is a smooth function such that \(\|\nabla \tilde{F}(x_1) - \nabla \tilde{F}(x_2)\| \leq L_c \|x_1 - x_2\|, \forall x_1, x_2 \in X\), where \(L_c := L_f + \frac{\|M_h\|L_h}{c} \|P_X\| + \frac{\|M_h\|^2}{c^2}, L_h := (L_{h1}, \cdots, L_{hm}), M_h := (M_{h1}, \cdots, M_{hm})\) and \(c > 0\).
Proof. Applying the first order optimality on \( \max_{y \in \mathbb{R}^n_+} f(x) + \langle h(x), y \rangle - \frac{1}{2} \| y \|^2 \) at \( y_{k-1} \) and \( y_k \), respectively, we obtain \( \forall y \in \mathbb{R}^n_+ \),

\[
\langle h(x_{k-1}) - cy_{k-1}, y - y_{k-1} \rangle \leq 0, \quad (A.4.7)
\]

\[
\langle h(x_k) - cy_k, y - y_k \rangle \leq 0. \quad (A.4.8)
\]

Furthermore,

\[
c\| y_{k-1} - y_k \|^2 \leq \langle h(x_{k-1}) - h(x_k), y_{k-1} - y_k \rangle \leq \| h(x_{k-1}) - h(x_k) \| \| y_{k-1} - y_k \| \leq M_h \| x_{k-1} - x_k \| \| y_{k-1} - y_k \|,
\]

where the first inequality is by summing up the two inequalities above with \( y \) replaced by \( y_h \) in (A.4.7) and \( y_{k-1} \) in (A.4.8); the second inequality follows from the Cauchy Schwarz inequality; the third one follows by the Lipschitz continuity of \( h \). This gives

\[
\| y_{k-1} - y_k \| \leq \frac{1}{c} M_h \| x_{k-1} - x_k \|.
\]

Next, we derive a bound for \( \| y_k \| \). Suppose \( x^* \) is an optimal solution of (1.1), then \( h(x^*) \leq 0 \). By (3.9) and the Lipschitz continuity of \( h(\cdot) \), we have

\[
\| y_k \| \preceq \| \max \left\{ \frac{h(x_k) - h(x^*)}{c}, 0 \right\} \| \leq \frac{\| h(x_k) - h(x^*) \|}{c} \leq \frac{M_h \| x_k - x^* \|}{c} \leq \frac{M_h \| D_x \|}{c}.
\]

Using the above inequality, the smoothness of \( f \) and \( h \), we arrive at

\[
\| \nabla \hat{F}(x_k) - \nabla \hat{F}(x_{k-1}) \|
\leq \| \nabla f(x_k) - \nabla f(x_{k-1}) + \langle y_k, \nabla h(x_k) \rangle - \langle y_k, \nabla h(x_{k-1}) \rangle + \langle y_k - y_{k-1}, \nabla h(x_{k-1}) \rangle \|
\leq \left( L_f + y_k^T L_h + \frac{M_h^2}{c} \right) \| x_{k-1} - x_k \|
\leq \left( L_f + \frac{M_h \| L_h \| D_x}{c} + \frac{M_h^2}{c} \right) \| x_{k-1} - x_k \|.
\]

\( \square \)

**Theorem 3.2** The total number of iterations required to compute an approximate solution \( \bar{x} \) such that \( Q(\bar{x}) \leq \epsilon \) and \( \| [h(\bar{x})]_+ \|^2 \leq \epsilon \) is bounded by \( \mathcal{O}(1/\epsilon^4) \).

Proof. Suppose \( \{ x_k \} \) is generated by Algorithm 4. Let \( \hat{F}^* := \min_{x \in X} \hat{F}(x) \), \( \hat{k} := \arg\min_{0 \leq k \leq K-1} Q(x_k) \), \( c = \frac{1}{K^{1/4}} \) and \( \alpha_k = \frac{1}{\sqrt{K}} \), where \( K \) is a known priori. By Lemma 3.1, we have

\[
\hat{F}(x_k) - \hat{F}(x_{k-1}) \leq \langle \nabla \hat{F}(x_{k-1}), x_k - x_{k-1} \rangle + \left( L_f + \frac{M_h \| L_h \| D_x}{c} + \frac{M_h^2}{c} \right) \| x_{k-1} - x_k \|^2.
\]

Since by the definition of \( Q(\cdot) \) and (3.8),

\[
\langle \nabla \hat{F}(x_{k-1}), x_k - x_{k-1} \rangle = \alpha_k \langle \nabla \hat{F}(x_{k-1}), p_k - x_{k-1} \rangle = -\alpha_k Q(x_{k-1}),
\]

we conclude that

\[
\hat{F}(x_k) - \hat{F}(x_{k-1}) \leq \frac{1}{\sqrt{K}} \left( L_f + \frac{M_h \| L_h \| D_x}{c} + \frac{M_h^2}{c} \right) \| x_{k-1} - x_k \|^2.
\]
then we have
\[
\alpha_k Q(x_{k-1}) \leq -\tilde{F}(x_k) + \tilde{F}(x_{k-1}) + \left( L_f + \frac{\|M_h\|\|L_h\|D_X}{c} + \frac{\|M_h\|^2}{c} \right) \alpha_k^2 \|x_{k-1} - p_k\|^2.
\]

Summing up the above inequality from \( k = 1 \) to \( K \) and using the fact that \( \tilde{F}^* \leq \tilde{F}(x_K) \) result in
\[
\left( \sum_{k=1}^{K} \alpha_k \right) \min_{1 \leq k \leq K} Q(x_{k-1}) \leq \tilde{F}(x_0) - \tilde{F}^* + \left( L_f + \frac{\|M_h\|\|L_h\|D_X}{c} + \frac{\|M_h\|^2}{c} \right) \sum_{1 \leq k \leq K} \alpha_k^2. \tag{A.4.9}
\]

Dividing both sides of (A.4.9) by \( \sum_{k=1}^{K} \alpha_k \), we obtain
\[
Q(x_k) \leq \frac{1}{\sqrt{K}} \left[ \tilde{F}(x_0) - \tilde{F}^* + \frac{L_f}{2} D_X^2 \right] + \frac{1}{K^{1/4}} \left( \frac{\|M_h\|^2 D_X^3}{2} + \frac{\|M_h\|\|L_h\|D_X^3}{2} \right). \tag{A.4.10}
\]

Next, we derive a bound for \( ||[h(x_k)]_+||^2 \). Let \( y_{ki} \) be the \( i \)-th element of the vector \( y_k \) at iteration \( k = 1, \cdots, K \). Note first, if \( h(x_k) \leq 0 \), then \( ||[h(x_k)]_+||^2 = 0 \). The analysis below focuses on the case where \( h(x_k) > 0 \). Consequently, by (3.9), we have \( y_{ki} = \frac{h(x_k)}{c} \), \( i = 1, \cdots, m \) and
\[
\sum_{i=1}^{m} y_{ki} h_i(x_k) = \sum_{i=1}^{m} \frac{1}{c} (h_i(x_k))^2. \tag{A.4.11}
\]

Note also, using the Lipschitz continuity and the lower curvature property of \( f \), it can be easily verified that
\[
\langle \nabla f(y), x - y \rangle \leq \frac{L_f}{2} D_X^2 + M_f D_X, \forall x, y \in X. \tag{A.4.12}
\]

Suppose \( x^* \) is the optimal solution of (1.1), then \( h(x^*) \leq 0 \). By convexity of \( h(\cdot) \) and the definition of \( Q(x_k) \) in (3.10), we obtain
\[
\sum_{i=1}^{m} y_{ki} h_i(x_k) \leq \sum_{i=1}^{m} y_{ki} (h_i(x^*) + \langle \nabla h_i(x_k), x_k - x^* \rangle)
\]
\[
\leq \sum_{i=1}^{m} y_{ki} \langle \nabla h_i(x_k), x_k - x^* \rangle
\]
\[
\leq Q(x_k) + \langle \nabla f(x_k), x^* - x_k \rangle
\]
\[
\leq Q(x_k) + \frac{L_f}{2} D_X^2 + M_f D_X,
\]
where the first inequality is because of the convexity of \( h(\cdot) \), the second inequality is due to \( h(x^*) \leq 0 \) and \( y_k \geq 0 \), the third inequality is by the definition of \( Q(x_k) \) and the last inequality follows from (A.4.12). Combining (A.4.11) and (A.4.13), we have
\[
||[h(x_k)]_+||^2 \leq c \left( Q(x_k) + \frac{L_f}{2} ||x^* - x_k||^2 + f(x^*) - f(x_k) \right)
\]
\[
\leq \frac{1}{K^{1/4}} \left( Q(x_k) + \frac{L_f}{2} D_X^2 + M_f D_X \right),
\]
which implies
\[
\|h(x_k)\| \leq \frac{1}{K^{3/4}} \left[ \tilde{F}(x_0) - \tilde{F}^* + \frac{L_f D_X^2}{2} \right] + \frac{1}{\sqrt{K}} \left( \frac{\|M_h\|^2 D_X^4}{2} + \frac{\|M_h\|\|L_h\| D_X^3}{2} \right) + \frac{1}{K^{1/4}} \frac{L_f}{2} D_X^3.
\] 
(A.4.14)

Combining (A.4.10) and (A.4.14), given target accuracy \( \epsilon > 0 \), the iteration complexity of DNCG of solving for \( \bar{x} \) such that \( Q(\bar{x}) \leq \epsilon \) and \( \|h(\bar{x})\| \leq \epsilon \) is bounded by \( O(1/\epsilon^4) \).

**Remark A.4.1.** In establishing the convergence rate of the DNCG method, we assume that \( h(\cdot) \) is a smooth function. Consider now when \( h(\cdot) \) is nonsmooth and inherits special structure as described in (A.1.17). Similar to Appendix A.1.3, we can apply Nesterov smoothing scheme and construct \( \{h_{i,\eta_i}\} \) such as
\[
h_{i,\eta_i}(x) := \max_{z \in Z_i} \left\{ \langle B_i x, z \rangle - \bar{h}_i(z) - \eta_i U_i(z) \right\}, \quad i = 1, \ldots, m.
\] (A.4.15)

In this way, \( h_{i,\eta_i}(x) \) is a \( L_{h_{i,\eta_i}} \)-smooth function with \( L_{h_{i,\eta_i}} = \frac{\|B_i\|^2}{\omega_i + \eta_i} \). We thereby define the gap function as \( Q_{\eta}(\tilde{x}) := \max_{x \in X} \langle \nabla \tilde{F}_\eta(\tilde{x}), x - \tilde{x} \rangle \), where \( \tilde{F}_\eta(x) = f(x) + \sum_{i=1}^m \eta_i h_{i,\eta_i}(x) - \frac{\xi}{2} \|y\|^2 \). Let \( \eta_i = \frac{\|M_{\eta_i}\|^2 D_X^4}{K^{1/4}} \), \( \forall i = 1, \ldots, m \). Then by Theorem 3.2, we have that \( Q_{\eta}(\tilde{x}) \) is upper bounded by \( O(1/K^3) \). By the second relation in (A.1.18), we have that \( \|h(x_k)\| \) is upper bounded by \( O(1/K^4) \).

**A.5. Auxiliary Numerical Studies**

**A.5.1. Portfolio Selection Models**

**Cardinality-free Models.** The objective function in model (Card-Free-Nonconvex) is a step function, which is discontinuous and nonconvex. To implement the proposed algorithms solving the model (Card-Free-Nonconvex), we employ a nonconvex smooth approximation of \( f(x) \) parameterized with \( \theta \) such as \( \tilde{f}_\theta(x) = \frac{1}{K} \sum_{k=1}^K \sum_{i \in \{1, \ldots, K\}} \frac{1}{1+\exp(-r_k z_i - \frac{1}{2} r_k z_i \theta)} \). Clearly, \( \tilde{f}_\theta \to f \) when \( \theta \to 0 \).

Now we discuss how to approximate the nonconvex model (Card-Free-Nonconvex) using the convex formulation. Define \( \phi(x) := [1 + x]_+ \). Since for some \( t > 0 \), \( \phi(tx) \geq 1 \), then for a random variable \( X \), we have
\[
\inf_{t > 0} E[\phi(tx)] \geq E[1_{\{X > 0\}}].
\] (A.5.1)

Consequently, instead of minimizing \( E[1_{\{X > 0\}}] \), we minimize its upper bound \( \inf_{t > 0} E[\phi(tx)] \), which is equivalent to minimizing \( \inf_{t > 0} \mathbb{E}[\phi(tX)] - \alpha \), where \( \alpha \) can be regarded as some confidence level such that \( \alpha > 0 \). Note that
\[
\inf_{t > 0} \mathbb{E}[\phi(tX)] - \alpha = \inf_{u \in \mathbb{R}} \{ u + \alpha^{-1} \mathbb{E}[X - u]_+ \}
\]
and the minimum of the right-hand-side of the above inequality falls in \([u, \bar{u}]\), where \( u \) and \( \bar{u} \) are the respective left and right side \( 1 - \alpha \) quantile of the distribution of \( X \). Coincidentally, \( \inf_{u \in \mathbb{R}} \{ u + \alpha^{-1} \mathbb{E}[X - u]_+ \} \) is the Conditional-Value-at-Risk (CVaR) measure that is convex. Leveraging such approximation, we arrive at the convex approximation of the nonconvex model in (Card-Free-Convex).
Cardinality-constrained Models. In model (Card-Nonconvex-2), to make the objective function continuous, we use the smooth approximation function \( \frac{1}{\Phi} \sum_{i=1}^{N} \frac{1}{1+\exp\left(-x_i/\theta\right)} \) to replace the step function in implementation.

A.5.2. IMRT Models

We provide more details in modeling the IMRT problem in this subsection. To elaborate, for each patient, the target body structures are discretized into small voxels \( v \) and the collection of all voxels is denoted by \( \mathcal{V} \). In the linac, each angle \( a \in A \) contains rectangular grids of beamlet \((l, r)\), \( l = 1, \ldots, m \), \( r = 1, \ldots, n \), which can stay active or blocked. An aperture \( e \in E_a \) of an angle \( a \) is then determined by the status of the beamlets. A set of binary variables \( \{x^{a,e}_{l,r}\} \) are created to decide the shape of the aperture \( e \) from angle \( a \). Specifically, \( x^{a,e}_{l,r} = 1 \) if beamlet \((l, r)\) is active, and \( x^{a,e}_{l,r} = 0 \) if beamlet \((l, r)\) is blocked. An additional set of variables \( \{y_{a,e}\} \) are created to decide the intensity rate of the selected aperture \( e \), where \( e \in E_a \). The unit intensity delivered to voxel \( v \) from beamlet \((l, r)\) is denoted by \( D(l, r)_v \) in Gy. Then the total amount of radiation received by voxel \( v \) is

\[
 z_v = \sum_{a \in A} \sum_{e \in E_a} \sum_{l=1}^{m} \sum_{r=1}^{n} RD(l, r)_v x^{a,e}_{l,r} y_{a,e}, \forall v \in \mathcal{V}.
\]

We use \( k \) to index the underdose/overdose clinical criteria, where \( k \in K_u(k \in K_o) \) denote the underdose (overdose) criterion and \( S_k \) to denote the set of structures in criterion \( k \), where \( S_k \subset \mathcal{V}, k \in K_u \cup K_o \). Additionally, we denote the number of voxels in \( \mathcal{V} \) by \( N_v \), the number of voxel in \( S_k \) by \( N_k \) and the required quantile of criterion \( k \) by \( p_k \).

Convex Formulation. Note that the left hand side in both (4.4) and (4.5) are nonconvex and we use CVaR for approximation in the convex formulation stated below. Follow the description in (Lan et al. 2021), the convex model is adapted as follows:

\[
 \min f(z) := \frac{1}{N_v} \sum_{v \in \mathcal{V}} w_v \left[ T_v - z_v \right]^2 + w_v \left[ z_v - T_v \right]^2
\]

s. t. \(-\tau_k + \frac{1}{p_k N_k} \sum_{v \in S_k} \left[ \tau_k - z_v \right]_+ \leq -b_k, \forall k \in K_u,\) \hspace{1cm} (A.5.3)

\[
 \tau_k + \frac{1}{p_k N_k} \sum_{v \in S_k} \left[ z_v - \tau_k \right]_+ \leq b_k, \forall k \in K_o,\)

\[
 z_v = \sum_{a \in A} \sum_{e \in E_a} \sum_{l=1}^{m} \sum_{r=1}^{n} RD(l, r)_v x^{a,e}_{l,r} y_{a,e}, \forall v \in S_k, k \in K_u \cup K_o,\) \hspace{1cm} (A.5.5)

\[
 \sum_{a \in A} \max_{e \in E_a} y_{a,e} \leq \Phi,\)

\[
 \sum_{a \in A} \sum_{e \in E_a} y_{a,e} \leq 1,\)

\[
 y_{a,t} \geq 0,\) \hspace{1cm} (A.5.8)
\[ \tau_k \leq \bar{\tau}_k, \ k \in K_u \cup K_o, \quad (A.5.9) \]
\[ \tau_k \geq \underline{\tau}_k, \ k \in K_u \cup K_o. \quad (A.5.10) \]

The objective function \( f(z) \) in (A.5.2), serving as a convex surrogate of the clinical criteria, penalizes underage and overage dose of a voxel with pre-defined threshold \( \bar{T}_v, \bar{\bar{T}}_v \) and weights \( w_v, \bar{w}_v \), where \( [\cdot]_+ \) denotes \( \max(\cdot, 0) \). To reinforce the clinical criteria, constraints (A.5.3) and (A.5.4) are added. To solve the convex model by the LCG method, smoothing scheme (with entropy distance generating function) is applied on all nonsmooth functionals ((A.5.3),(A.5.4) and (A.5.6)), which includes construction of \( \{h_{i,n}\} \) as indicated in Algorithm 5 for nonsmooth underdose/overdose constraints and the group sparsity constraint.

**Nonconvex Formulation.** The exact nonconvex formulation is described as follow.

\[
\begin{align*}
\min f(z) &:= \sum_{k \in K_u} w_k \frac{1}{N_k} \sum_{v \in S_k} 1_{(z_v < \tau_k)} + \sum_{k \in K_o} w_k \frac{1}{N_k} \sum_{v \in S_k} 1_{(z_v > \tau_k)} \\
\text{s.t. } z_v & = \sum_{a \in A} \sum_{e \in E_a} \sum_{l=1}^{m} \sum_{r=1}^{n} RD_{(l,r)v} x_{l,r}^{a,e} y_{a,e}, \ \forall v \in S_k, k \in K_u \cup K_o, \\
\sum_{a \in A} \max_{e \in E_a} y_{a,e} & \leq \Phi, \\
\sum_{a \in A} \sum_{e \in E_a} y_{a,e} & \leq 1, \\
y_{a,e} & \geq 0.
\end{align*}
\] (A.5.11)

Here \( \{w_k\} \) is a set of weights for underdose and overdose objective terms; \( f(\cdot) \) is a step function which is nonconvex and discontinuous; \( \{\tau_k\} \) are parameters given by the clinical criteria, instead of decision variables to calibrate the approximation in the case of the convex formulation. To solve the model by the proposed algorithm, we employ a sigmoid function (parameterized on \( \theta \)) to approximate the original function. Specifically, for \( k \in K_u \), the approximation reads

\[ \tilde{f}_\theta^k(x) = \frac{1}{N_k} \sum_{v \in S_k} \frac{1}{1 + \exp\{(z_v - \tau_k)/\theta\}}. \] (A.5.12)

Similarly, for \( k \in K_o \),

\[ \tilde{f}_\theta^k(x) = \frac{1}{N_k} \sum_{v \in S_k} \frac{1}{1 + \exp\{(-z_v + \tau_k)/\theta\}}. \] (A.5.13)

Note that when \( \theta \to 0 \), \( \tilde{f}_\theta \to f \) and \( \tilde{f}_\theta \) is nonconvex.

**A.5.3. IMRT Synthetic Dataset**

The synthetic dataset used in Section 4 mimics the IMRT dataset of a real patient, with each containing information of (discretized) voxels, beamlet coordinates and corresponding unit intensity \( (D \text{ matrix}) \) received by each voxel. In particular, each angle pairs with a \( D \) matrix with dimension
of \# of voxels \times \# of beamlets, and there are 180 \( D \) matrices in total. In particular, the number of beamlets is determined by the discretization granularity (beamlet unit length).

Table A.1 describes main features of each dataset, where “Granularity” stands for beamlet unit length. Instance 1 and 2 (resp. instance 3 and 4) are featured in lower (resp. higher) beamlet granularity and have the same set of \( D \) matrices and voxels. Higher discretization accuracy (e.g. 0.25) results in larger number of beamlets, thus in higher dimension of \( D \) matrix. Therefore, instance 3 and 4 are in larger scale than instance 1 and 2. Among all the voxels, we randomly select two sets of tumor tissues that require radiation therapy and treat the rest as the healthy ones. For the tumor issues, we consider two underdose and one overdose constraints.

| Instance | # of angels | # of voxels | # of beamlets | Accuracy | \( b_k \)      | \( p_k \)       |
|----------|-------------|-------------|---------------|----------|----------------|----------------|
| 1        | 180         | 4096        | 100           | 1.0      | [40, 50, 100]  | [0.01, 0.01, 0.05] |
| 2        | 180         | 4096        | 100           | 1.0      | [50, 60, 80]   | [0.01, 0.01, 0.01] |
| 3        | 180         | 262144      | 2000          | 0.25     | [40, 50, 100]  | [0.01, 0.01, 0.05] |
| 4        | 180         | 262144      | 2000          | 0.25     | [50, 60, 80]   | [0.01, 0.01, 0.01] |

### A.5.4. Auxiliary Results on IMRT Synthetic Dataset

Table A.2 displays the results of applying LCG to solve the convex formulation (A.5.2) - (A.5.10) with various \( \Phi \). From the table, we observe that regardless of the large difference in scale among the instances, the proposed algorithm LCG exhibits comparable performance in solving all instances in view of the objective value and constraint violation at iteration 1000. By comparing instance 1 and instance 2 (namely, instance 3 and instance 4), we see that the values of \( \|h(x_N)\|_2 \) in instance 1 (resp. instance 3) remain lower than those in instance 2 (resp. instance 4). Such results indicate that the satisfaction of the constraints are sensitive to the choice of \( (b_k, p_k) \) thus to the decision variable \( \tau_k \), which jointly determine the CVaR approximation. An additional observation is that when \( \Phi \) decreases (i.e. sparsity requirement is more stringent), the violation of the group sparsity constraint increases, which is an expected effect of \( \Phi \).
### Table A.2 Results of applying LCG on the synthetic dataset at iteration 1000.

| Instance | $\Phi$ | $f(x_N)$ | $\|h(x_N)\|_2$ | $\|h_s\|_2$ | $\|h_c\|_2$ | Time (s) |
|----------|-------|----------|-----------------|--------------|--------------|-----------|
| 1        | 1.0   | 0.0136   | 0.319           | 0            | 0.319        | 901       |
|          | 0.5   | 0.0142   | 0.326           | 0            | 0.326        | 914       |
|          | 0.05  | 0.0156   | 0.449           | 0.302        | 0.332        | 948       |
|          | 0.005 | 0.0193   | 0.528           | 0.421        | 0.319        | 924       |
|          | 0.0005| 0.0174   | 0.576           | 0.499        | 0.288        | 938       |
| 2        | 1.0   | 0.0156   | 0.626           | 0            | 0.626        | 916       |
|          | 0.5   | 0.0161   | 0.628           | 0            | 0.628        | 923       |
|          | 0.05  | 0.0197   | 0.702           | 0.291        | 0.639        | 942       |
|          | 0.005 | 0.019   | 0.763           | 0.402        | 0.649        | 908       |
|          | 0.0005| 0.0142   | 0.815           | 0.476        | 0.662        | 949       |
| 3        | 1.0   | 0.0479   | 0.434           | 0            | 0.434        | 4678      |
|          | 0.5   | 0.0466   | 0.436           | 0            | 0.436        | 4726      |
|          | 0.05  | 0.0514   | 0.451           | 0.087        | 0.442        | 4685      |
|          | 0.005 | 0.0473   | 0.476           | 0.169        | 0.445        | 4834      |
|          | 0.0005| 0.048    | 0.493           | 0.188        | 0.456        | 4842      |
| 4        | 1.0   | 0.0421   | 0.919           | 0            | 0.919        | 4766      |
|          | 0.5   | 0.0441   | 0.943           | 0            | 0.943        | 4762      |
|          | 0.05  | 0.0498   | 0.969           | 0.068        | 0.967        | 4813      |
|          | 0.005 | 0.0435   | 0.984           | 0.175        | 0.968        | 4871      |
|          | 0.0005| 0.0433   | 0.975           | 0.201        | 0.954        | 4772      |