Discrete Convex Simulation Optimization

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We propose new sequential simulation algorithms for general convex simulation optimization problems with high-dimensional discrete decision space. The performance of each discrete decision variable is evaluated via stochastic simulation replications. Our proposed simulation algorithms utilize the discrete convex structure and are guaranteed with high probability to find a solution that is close to the best within any given user-specified precision level. The proposed algorithms work for any general convex problem and the efficiency is demonstrated by proved upper bounds on simulation costs. The upper bounds demonstrate a polynomial dependence on the dimension and scale of the decision space. For some discrete simulation optimization problems, a gradient estimator may be available at low costs along with a single simulation replication. By integrating gradient estimators, which are possibly biased, we propose simulation algorithms to achieve optimality guarantees with a reduced dependence on the dimension under moderate assumptions on the bias.

Key words: Discrete simulation optimization, discrete convex functions, sequential simulation algorithms, simulation costs, biased gradient estimators

1. Introduction

Many decision making problems in operations research and management science involve large-scale complex stochastic systems. The objective function in the decision making problems often involve expected system performances that need to be evaluated by discrete-event simulation or general stochastic simulation. The decision variable in many of these problems is naturally discrete
and multi-dimensional. This class of problems is also called discrete optimization via simulation; see Nelson (2010), Hong et al. (2015) and Salemi et al. (2019). Typically for discrete simulation optimization problems, continuous approximations are either not naturally available or may incur additional errors that are themselves difficult to accurately quantify. This work is centered around designing and proving theoretical guarantees for simulation algorithms to solve simulation optimization problems with discrete and high-dimensional decision space.

In large-scale complex stochastic systems, one replication of simulation to evaluate the performance of a single decision variable can be computationally costly. An accurate evaluation of the expected performance associated with a single decision variable need many independent replications of simulation. Running simulations for all decision variables in a high-dimensional discrete space to find the optimal is computationally prohibitive. The use of parallel computing (Luo et al. (2015)) alleviates the situation, but to find the best decision in high-dimensional problems can still be challenging. Fortunately, for a number of applications, the objective function exhibits convexity in the discrete decision variables, or the problem can be transformed into a convex one. One such example with convex structure comes from the bike-sharing system (Singhvi et al. 2015, Jian et al. 2016, Freund et al. 2017). This problem involves around 750 stations and 25000 docks (Singhvi et al. 2015). The goal is to find the optimal allocation of bikes and docks, which are naturally discrete decision variables. The performance of each allocation is evaluated by the dissatisfaction function, which is defined as the total number of failures to rent or return a bike in a whole day. In presence of non-stationary random demands and travel patterns, the evaluation of the dissatisfaction function for a given allocation needs to be done by simulation. This simulation is costly as it may need to simulate the full operation of the system over the entire day. In Freund et al. (2017), the expected dissatisfaction function is proved to be “convex” under a linear transformation if the sequences of arrivals are exogenous. For this problem, the decision space is discrete and high-dimensional. Utilizing the convex structure to reduce the dependence of computation complexity on dimension is important. Freund et al. (2017) propose an algorithm for the deterministic case, which may fail
to produce statistically guaranteed results in the stochastic case. Many performance functions in the operations research and management science domain also exhibit convexity in discrete decision variables. For example, the expected customer waiting time in a multi-server queueing network were proved to be convex in the routing policy and staffing decisions; see Altman et al. (2003) and Wolff and Wang (2002). Shaked and Shanthikumar (1988) discuss a wide range of stochastic systems including queueing systems, reliability systems and branching systems and show convexity of key expected performance measures as a function of the associated decision variable. In addition, a large variety of problems in economics, computer vision and network flow optimization exhibit convexity with discrete decision variables (Murota 2003).

Even in presence of convexity, the nominal task in discrete simulation optimization – correctly finding the best decision variable with high enough probability, which is often referred to as the Probability of Correct Selection (PCS) guarantee – can still be computationally prohibitive. For a convex problem without convenient assumptions such as strong and strict convexity, there may be a large number of decision variables that render very close objective value compared to the optimal. In this case, the simulation efforts to identify the exact optimal decision variable can be huge and practically unnecessary. Our focus, alternatively, is to find a good decision variable that is assured to render $\epsilon$-close objective value compared to the optimal with high probability, where $\epsilon$ is any arbitrary small user-specified precision level. This guarantee is also called the Probability of Good Selection (PGS) or Probably Approximately Correct (PAC) in the literature. This paper adopts the notion of PGS as a guarantee for simulation algorithms design. We refer to Eckman and Henderson (2018a) and Eckman and Henderson (2018b) for thorough discussions on settings when the use of PGS is preferable compared to the use of PCS. In this work, we propose simulation algorithms that achieve the PGS guarantee for general discrete convex problems, without knowing any further information such as strong convexity etc. Knowing strong convexity or a specific parametric function form of the objective function, of course, will enhance the simulation algorithms. However, such fine structural information may not be available a priori for large-scale
simulation optimization problems. The design of our simulation algorithms utilize the convex structure and the intuition is that the convex structure of optimization landscapes can provide global information through local evaluations. Global information avoids the algorithm from evaluating all feasible decision solutions, which may result in simulation efforts that are proportional to the number of feasible decision solutions and are exponentially dependent on the dimension in general. The proposed simulation algorithms are based on stochastic gradient methods and discrete steepest descent methods, which have fundamental difference compared to continuous optimization algorithms. For high-dimensional problems, gradient-based methods are preferred compared to strongly polynomial methods like cutting-plane methods, because gradient-based methods have lighter dependence of simulation costs on the dimension.

Besides the PGS optimality guarantee, the running time is an important characteristic of simulation algorithms. In general, the running time of simulation algorithms provides a clue or an upper bound to the difficulty of given class of simulation problems. Also, estimating the running times of simulation algorithms helps determining the computational resources needed for producing a suitable solution. The running time also serves as a measurement to compare different simulation algorithms that achieve the same optimality guarantee; see also [Ma and Henderson (2019)] for supportive discussions. In this paper, we do not distinguish the difference in simulation cost for different decision variables, and we evaluate the running time by the expected simulation costs, i.e., the expected number of replications of simulations that are run. We prove upper bounds on the expected simulation cost for our proposed simulation algorithms that achieve the PGS guarantee. The upper bound on expected simulation cost holds for any convex problem that is sent to the simulation algorithm. (Instead, if the target is to select the best system, the expected simulation cost for any algorithm can be arbitrarily large, and there exists no upper bound on expected simulation cost for an algorithm that works for all convex problems.) The upper bound demonstrates a quadratic dependence on the decision space dimension $d$, which are of key interest for high-dimensional large-scale problems. As a comparison, if the convex structure is not present or
utilized, the simulation costs to achieve PGS guarantee can be exponential in the dimension $d$.

We also provide lower bounds on the expected simulation costs that are needed for any possible simulation algorithm. The lower and upper bounds of expected simulation costs imply the limit of algorithm performance and provide directions to improving existing simulation algorithms.

In large-scale discrete simulation optimization, during a simulation run with a given $d$-dimensional decision variable $x$, it is sometimes possible that the neighboring decision variables can be evaluated simultaneously within the same simulation run for $x$. When the decision variable $x$ is in continuous space, this simultaneous simulation approach is called the Infinitesimal Perturbation Analysis (IPA) or the Forward/Backward Automatic Differentiation. Such gradient estimators can be unbiased under Lipschitz continuity regularity conditions, though no guarantees on bias exist for general conditions. In contrast, for discrete simulation optimization problems, in particular those where discrete decision variables do not easily relax to continuous variables, the gradient information becomes the difference of function value on $x$ and function value on the neighboring points of $x$. This gradient information is very difficult to obtain without bias, if not impossible, within only a single simulation run. In general, the system dynamics and logic can be different even for two discrete decision variables with difference only in one coordinate. Therefore, in the simulation run for decision variable $x$, the simultaneous evaluation for neighbor decision variables may incur a bias. See Chapter 4 of Jian (2017) for an example in the bike-sharing simulation optimization. Despite of the bias, the benefit of having gradient information at marginal costs is significant when $d$ is large. We design simulation algorithms that utilize the biased gradient information to achieve the PGS guarantee.

1.1. Main Results and Contributions

We design gradient-based simulation algorithms that achieve PGS guarantee for general discrete convex problems with high-dimensional and large-scale decision space. We consider the decision space to be $\{(x_1, x_2, \ldots, x_d) : x_i \in \{1, 2, \ldots, N\}, i \in \{1, 2, \ldots, d\}\}$ that has in total $N^d$ decision variables. The discrete convexity in high dimension that preserves the mid-point convexity is called
L₂-convexity (Murota 2003). From the optimization perspective, our work addresses the stochastic version of discrete convex analysis in Murota (2003). From the simulation optimization perspective, this work provides simulation algorithms with optimality guarantee and polynomial dependence of simulation costs on dimension, for high-dimensional discrete convex simulation optimization problems.

We differentiate our simulation algorithms to two classes. One class is the \textit{Zero-order Algorithm}, for which the simulation is a black-box and one run of simulation can only provide an evaluation of a single decision variable. The other class is the \textit{First-order Algorithm}, for which the neighboring decision variables can be simultaneously evaluated (possibly with bias) within a single simulation run for a given decision variable. We develop simulation algorithms with PGS guarantee as a major focus, but we also provide algorithms with PCS-IZ guarantee for cases when the indifference zone (IZ) parameter is known. See Hong et al. (2020) for detailed discussions on the PCS-IZ guarantee. We summarize our results in Table 1 where algorithm performance is demonstrated by the expected simulation cost. In this table, we omit terms in the expected simulation cost that do not depend on the failing probability $\delta$. Therefore, when $\delta$ is very small, the dominating term in the expected computation cost is what we list in Table 1. This comparison scheme is also considered in Kaufmann et al. (2016). That being said, we provide all terms in the upper bounds for expected simulation costs in corresponding theorems.

For zeroth-order algorithms, the Lovász extension (Lovász 1983) is introduced to define a convex linear interpolation of the original discrete function. Using properties of the Lovász extension (Fujishige 2005), we equivalently optimize the continuous interpolated function. Therefore the projected stochastic subgradient descent method can be used to find PGS solutions. Also, the truncation of stochastic subgradients is essential in reducing the expected simulation costs and we prove that the dependence on dimension $d$ is reduced from $O(d^3)$ to $O(d^2)$ using truncation. In stochastic optimization literature, it is common to assume the stochastic subgradient is bounded when deriving high-probability bounds. Even though in the general simulation context the boundedness assumption on stochastic subgradients is hard to verify, we provide a theoretical guarantee...
Table 1 Upper bounds on expected simulation cost for the proposed simulation algorithms that achieve the PGS and PCS-IZ guarantees. Constants except $d, N, \epsilon, \delta, c$ are omitted in the $O(\cdot)$ notation. In comparison, the expected simulation cost without $L^3$-convexity is $O(N^d\epsilon^{-2}\log(1/\delta))$.

| Algorithms                  | PGS                  | PCS-IZ (known IZ parameter $c$) |
|-----------------------------|----------------------|---------------------------------|
| Zeroth-order Alg. (Gaussian Noise) | $O(d^2N^2\epsilon^{-2}\log(1/\delta))$ | $O(d^2\log(N)c^{-2}\log(1/\delta))$ |
|                            | (Lower bound: $O(d\epsilon^{-2}\log(1/\delta))$) |                                 |
| Zeroth-order Alg. (Assumption 6) | $O(dN^2\epsilon^{-2}\log(1/\delta))$ | $O(d\log(N)c^{-2}\log(1/\delta))$ |
| Unbiased First-order Alg. (Assumption 7) | $O(dN^2\epsilon^{-2}\log(1/\delta))$ | $O(d\log(N)c^{-2}\log(1/\delta))$ |
| Biased First-order Alg. (Assumption 8) | $O(N^3\epsilon^{-2}\log(1/\delta))$ | $O(Nc^{-2}\log(1/\delta))$ |
|                            | (requires additional memory cost) |                                 |

as a complement. When the boundedness assumption can be verified, the dependence on dimension can be further reduced to $O(d)$. When the indifference zone parameter $c$ is known, this additional knowledge does not reduce the the dependence of expected simulation cost on dimension. Instead, the information about indifference zone parameter can help reduce the dependence on the scale $N$. More specifically, an accelerated algorithm is proposed and is proved to reduce the dependence from $O(N^2)$ to $O(\log(N))$. Finally, an information-theoretical lower bound is derived to show the limit of simulation algorithms.

For first-order algorithms, we have available gradient information, at a cost as a constant multiplying the cost of one simulation run, for which the constant does not depend on the dimension. This gradient information is regarded as a subgradient estimator. If the subgradient estimator shares similar properties as stochastic subgradients, such as the unbiasedness and componentwise
independence, the stochastic subgradient method can still be applied and the expected simulation costs are reduced by $O(d)$. In practice, the subgradient estimator can be biased, and there is no convergence guarantee for any optimization algorithms in general. However, under a moderate assumption on the bias, we are still able to develop simulation algorithms that achieve the PGS guarantee through a stochastic version of steepest descent method. The associated simulation cost does not scale up with $d$, but the memory cost can be much larger than that of simulation algorithms designed for the unbiased gradient estimators. When the indifference zone parameter is known, the expected simulation cost is reduced by $O(N/\epsilon)$, where $\epsilon$ is the user-specified precision level. Finally, utilizing the indifference zone, the expected simulation cost can be reduced from $O(N^3)$ to $O(N)$ in terms of dependence on $N$.

1.2. Literature Review

The problem of selecting the best system or a good system through simulation has been widely studied in the simulation literature. The problem is often called the ranking-and-selection (R&S). We refer to Hong et al. (2020) as a recent review of this literature. There have been two approaches to categorize the R&S literature. One approach is differentiating the frequentist view and the Bayesian view when describing the probability models and procedures in R&S; see Kim and Nelson (2006) and Chick (2006). The other approach differentiates the fixed-confidence procedures and the fixed-budget procedures; see Hunter and Nelson (2017) and Hong et al. (2020). In particular, the probability of correct selection (PCS) of the best system has been a widely used guarantee for both types of procedures. For fixed-budget procedures, the R&S problem is usually formulated as a computation resource allocation problem with the goal of maximizing the PCS under a budget constraint; see Chen (1996), Chen et al. (2000), Chick and Inoue (2001), Frazier et al. (2009), Chen and Lee (2011), Peng et al. (2018), Wu and Zhou (2018) among others. Gao et al. (2017) consider a fixed-budget procedure but with a different guarantee called expected opportunity cost. Fixed-confidence procedures, on the other hand, develop simulation algorithms to deliver
the best system with a given PCS guarantee; see Kim and Nelson (2001), Kim (2005), Frazier (2014), Fan et al. (2016) among others.

A large number of R&S procedures based on PCS guarantee adopt the indifference zone formulation, called PCS-IZ. The PCS-IZ guarantee is built upon the assumption that the expected performance of the best system is at least $c > 0$ better than all other systems. This IZ parameter $c$ is typically assumed to be known, while Fan et al. (2016), as a notable exception, provide selection guarantees without the knowledge of the indifference-zone parameter. In practice, this IZ parameter is likely unknown a priori. When many systems have close performance compared to the best, it is practically inefficient to select the exact best. In this case, systems that are close enough to the best are referred to as “good systems” and any one of them can be satisfying. This naturally gives rise to a notion of probability of good selection (PGS). Eckman and Henderson (2018a) and Eckman and Henderson (2018b) have thoroughly discussed settings when the use of PGS is preferable compared to the use of PCS. Regarding the PGS guarantee, Ma and Henderson (2017) present a sequential selection procedure called the Envelope Procedure to ensure a PGS selection, when the variances for all systems are unequal and sequentially estimated.

Discussions on discrete optimization via simulation can be found in Fu (2002), Nelson (2010), Sun et al. (2014), Hong et al. (2015) and Chen et al. (2018) among others. Hu et al. (2007, 2008) have discussed model reference adaptive search algorithms in order to ensure global convergence. Hong and Nelson (2006), Hong et al. (2010), Xu et al. (2010) propose and study algorithms based on the convergent optimization via most-promising-area stochastic search (COMPASS) that can be used to solve general simulation optimization problems with discrete decision variables. The proposed algorithms are computationally efficient and are proved to convergence with probability one to optimal points. Lim (2012) study simulation optimization problems over multidimensional discrete sets where the objective function adopts multimodularity. They propose algorithms that converge almost surely to the global optimal. Wang et al. (2013) discuss stochastic optimization problems with integer-ordered decision variables. Park and Kim (2015) and Park et al. (2014)
develop and examine the Penalty Function with Memory (PFM) method for discrete optimization via simulation with stochastic constraints. Sun et al. (2014) discuss an exploration-exploitation balancing approach using Gaussian process based search. Eckman et al. (2020) discuss a statistically guaranteed screening to rule out decisions based on initial simulation experiments utilizing the convex structure.

When a simulation problem involves a response surface to estimate or optimize over, gradient information may be constructed and used to enhance simulation. Chen et al. (2013) construct gradient estimator to enhance simulation metamodeling. Qu and Fu (2014) propose a new approach called gradient extrapolated stochastic kriging that exploits the extrapolation structure. Fu and Qu (2014) discuss the use of Monte Carlo gradient estimators to enhance regression. See also L’Ecuyer (1990) for a review of Monte Carlo gradient estimators. Eckman and Henderson (2020) discusses the use of possibly gradient estimators in continuous stochastic optimization, by assuming that the bias is uniformly bounded. Wang et al. (2020) considers a setting in which the response surface is a quadratic function and gradient information is available and discusses optimal budget allocation to maximize PCS. In general simulation optimization problem, when the decision variable is discrete, the gradient with respect to the decision variable may not be appropriately defined. Instead, the difference of performance between two neighboring decision variables contains the gradient-like information. Jian (2017) uses this information to drive the search for the optimal decision variable.

Discrete simulation optimization is also formulated as the best-arm identification problem, or the pure-exploration multi-armed bandit problem. The best-arm identification problems usually do not consider the problem structure nor the high-dimensional nature of an arm. In the fixed-confidence best-arm identification setting, Even-Dar et al. (2002, 2006) give an elimination-based algorithm for bounded bandit models with the PGS guarantee, which is proved to be optimal by Mannor and Tsitsiklis (2004). Later, Kalvanakrishnan and Stone (2010), Kalvanakrishnan et al. (2012) extend the best-arm identification problem to the best \( k \) arms identification problem and develop UCB-based algorithms. Problem-dependent sample complexity is
improved in Karnin et al. (2013), Jamieson et al. (2014) by elimination-based and UCB-based algorithms, respectively. Also, Jamieson et al. (2014) proves that the improved bound is optimal when the difference between expectations of optimal and sub-optimal arms goes to zero. More recently, Chen et al. (2017) further narrows the gap between the problem-dependent lower bound and upper bound.

The aforementioned results for bounded or Gaussian bandit models are extended to sub-Gaussian bandit models. Recent works focus on more general distribution families by techniques from information theory. Informational upper bounds and lower bounds for exponential bandit models are established by the change of measure technique in Kaufmann and Kalvanakrishnan (2013), Kaufmann et al. (2016) for both the fixed-confidence and fixed-budget settings. For two-armed bandit models, a tighter lower bound is proposed in Kaufmann et al. (2014) and, when the distribution is bounded or Gaussian, a matching algorithm is given. In Garivier and Kaufmann (2016), a transportation inequality is proved and a general non-asymptotic lower bound can be formulated thorough the solution of a max-min optimization problem. In addition, an asymptotically optimal algorithm, named Track-and-Stop, is proposed for exponential bandit models in the same literature. The Track-and-Stop algorithm is further improved by Degenne et al. (2019), Degenne and Koolen (2019). Agrawal et al. (2020) shows that restrictions on the distribution family are necessary and generalizes the algorithm to models with milder restriction than exponential family.

In the fixed-budget setting, Bubeck et al. (2011) shows that algorithm for regret minimization is not suitable for the pure-exploration setting. In Audibert and Bubeck (2010), an asymptotic lower bound on the sample complexity is derived when the failing probability goes to zero. A highly exploring UCB-based method and an algorithm based on successive rejections are proposed in Audibert and Bubeck (2010), Bubeck et al. (2011), respectively. The gap between the upper and lower bound is closed in Carpentier and Locatelli (2016) and the successive rejection based algorithm is proved to be optimal. The results in the last paper also shows non-trivial difference between the fixed-confidence and fixed-budget settings. Yu et al. (2018) extends the results for
sub-Gaussian arms to a more general distribution family. In Russo (2020) and Qin et al. (2017), a Bayesian setting is studied and the posterior failing probability is proved to converge to zero with an optimal rate. We refer to Lattimore and Szepesvári (2020), Kaufmann et al. (2016) for a thorough review of the best-arm identification problem.

Simulation optimization problems fall into the more general class of problems called discrete stochastic optimization. In contrast to continuous optimization, works on discrete stochastic optimization Futschik and Pflug (1995), Gutjahr and Pflug (1996), Futschik and Pflug (1997), Kleywegt et al. (2002), Semelhago et al. (2020) do not consider the convex structure. The main obstacle to the development of discrete convex optimization lies in the lack of a suitable definition of discrete convex structure. A natural definition of discrete convex functions would be functions that are extensible to continuous convex functions. However, for that class of functions, the local optimality does not imply the global optimality and therefore the definition is not suitable for the purpose of optimization. Later, Favati (1990) proposes a stronger condition, named the integral convexity, that ensures the local optimality is equivalent to the global optimality. On the other hand, after Lovász (1983) shows the equivalence between the submodularity of a function and the convexity of its Lovász extension, submodular functions are viewed as the discrete analogy of convex functions in the field of combinatorial optimization. This idea is also solidified by the Fenchel-type min-max duality theorem by Fujishige (1984). Moreover, the Lovász extension along with the subgradient conceived in Fujishige (2005) provides a good framework of applying gradient-based method to the submodular function minimization (SFM) problem. The SFM problem has wide application in computer vision, economics, game theory and is well-studied in literature (Lee et al. 2015, Axelrod et al. 2020, Zhang et al. 2020). In contrast, the stochastic SFM problem is less understood and Ito (2019) gives the only result on stochastic SFM problem, where they provide upper and lower bounds for finding solutions with small error bound in expectation. In Bach (2019), Axelrod et al. (2020), the authors extend the domain of submodular function to $\{1,2,\ldots,N\} \times \cdots \{1,2,\ldots,N\}$ by requiring the submodular inequality at any pair of points,
and show that the generalized submodular function is equivalent to a submodular function on a sub-lattice of $\mathbb{Z}^{(N-1)d}$. In Murota (2003), an alternative generalization of submodular functions, called the $L^3$-convex functions, are defined through the translation submodularity. The $L^3$-convex functions are equivalent to functions that are both submodular and integrally convex on integer lattice. In addition, the $L^3$-convex function has a convex extension that shares similar properties as the Lovász extension and therefore gradient-based methods are also applicable for $L^3$-convex functions minimization. We refer readers to Murota (2003) for more discussion about discrete convex functions.

Also, we can view evaluations through simulation as stochastic zeroth-order oracles and therefore simulation algorithms can be viewed as zeroth-order optimization algorithms. The idea of approximating gradient using finite difference appeared as early as Nemirovsky and Yudin (1983). Nesterov and Spokoiny (2017) elaborate this idea to the Gaussian smoothing technique and derive bounds of zeroth-order methods on deterministic smooth and non-smooth convex problems. Later, Duchi et al. (2015) utilized this idea to design an optimal zeroth-order mirror descent method for stochastic convex problems. Furthermore, the RSGF method in Ghadimi and Lan (2013) also incorporates the Gaussian smoothing technique and gives the first bound on stochastic nonconvex smooth problems. In the follow-up work by Balasubramanian and Ghadimi (2018), the zeroth-order conditional gradient method is designed to handle the constrained case. In the same literature, a linear-time zeroth-order estimator of the Hessian matrix is proposed and is used to construct a saddle-point avoiding method, named the zeroth-order cubic regularization method. We refer readers to Homem-de Mello and Bayraksan (2014), Larson et al. (2019) for a review of recent developments for zeroth-order algorithms.

1.3. Notation

For $N \in \mathbb{N}$, we define $[N] := \{1, 2, \ldots, N\}$. For a given set $S$ and an integer $d \in \mathbb{N}$, the product set $S^d$ is defined as $\{(x_1, x_2, \ldots, x_d) : x_i \in S, i \in [d]\}$. For example, if $S = [N]$, then $S^d = \{(x_1, x_2, \ldots, x_d) : x_i \in \{1, 2, \ldots, N\}, i \in [d]\}$ in which $[d] = \{1, 2, \ldots, d\}$. For two vectors $x, y \in \mathbb{R}^d$, we use $(x \wedge y)_i := \min\{x_i, y_i\}$. In addition, if $S = \mathbb{N}$, then $S^d = \{(x_1, x_2, \ldots, x_d) : x_i \in \mathbb{N}, i \in [d]\}$. In this case, we use $(x \wedge y)_i := \min\{x_i, y_i\}$.
\[
\min\{x_i, y_i\} \quad \text{and} \quad (x \lor y)_i := \max\{x_i, y_i\}
\]
to denote the component-wise minimum and maximum. Similarly, the ceiling function \(\lceil \cdot \rceil\) and the flooring function \(\lfloor \cdot \rfloor\) round each component to an integer when applied to vectors. For a stochastic system labeled by its decision variable \(x\), we denote \(\xi_x\) as the random object associated with the system. We write \(\xi_{x,1}, \xi_{x,2}, \ldots, \xi_{x,n}\) as independent and identically distributed (iid) copies of \(\xi_x\). We use \(\hat{F}_n(x) \triangleq \frac{1}{n} \sum_{j=1}^{n} F(x, \xi_{x,j})\) to denote the empirical mean of the \(n\) independent evaluations for system labeled by \(x\). The notation \(f = O(g)\) (resp. \(f = \Theta(g)\)) means that there exist constants \(c_1, c_2, c_3 > 0\) independent of \(N, d, \epsilon, \delta, c\) such that \(f \leq c_1 g + c_3\) (resp. \(c_1 g \leq f \leq c_2 g + c_3\)). Similarly, the notation \(f = \tilde{O}(g)\) (resp. \(f = \tilde{\Theta}(g)\)) means that there exist constants \(c_1, c_2 > 0\) independent of \(N, d, \epsilon, \delta, c, \gamma\) and constant \(c_3 > 0\) independent of \(\delta\) such that \(f \leq c_1 g + c_3\) (resp. \(c_1 g \leq f \leq c_2 g + c_3\)). In other words, we omit terms that are independent of \(d, N, \epsilon, \delta, c, \gamma\) in \(O(\cdot), \Theta(\cdot)\) and omit terms independent of \(\delta\) in \(\tilde{O}(\cdot), \tilde{\Theta}(\cdot)\).

2. Model and Framework

The model in consideration contains a complex stochastic system whose performance depends on discrete decision variables that belong to a \(d\)-dimensional subspace \(\mathcal{X} = [N_1] \times [N_2] \times \cdots \times [N_d]\) in which the \(N_i\)'s are positive integers. From a modeling perspective, in a stochastic system, the system performance may depend on three elements: the decision variable \(x \in \mathbb{Z}^d\), a random object \(\xi_x\) supported on a proper space \((\mathcal{Y}, \mathcal{B}_\mathcal{Y})\) that summarizes all the associated random quantities and processes involved in the system when the decision \(x\) is taken, and a deterministic function \(F: \mathcal{X} \times \mathcal{Y} \to \mathbb{R}\) that takes the decision variable and a realization of the randomness as inputs and outputs the associated system performance. Specifically, the deterministic function \(F\) captures the full operations logic of the stochastic system that can be complicated. The objective function with decision variable \(x\) is given by

\[
f(x) := \mathbb{E}[F(x, \xi_x)].
\]

We consider scenarios when \(f(x)\) does not adopt a closed-form representation and can only be evaluated by averaging over simulation samples of \(F(x, \xi_x)\). The selection of a good system is
through the selection of a decision variable $x$ that renders a better objective value $f(x)$. Denote $x^*$ as any decision variable that renders the optimal objective value, such that

$$f(x^*) = \min_{x \in \mathcal{X}} f(x).$$

(1)

Note that we fix the use of minimum operation to represent the optimal. Our general goal is to develop simulation algorithms that select a good decision variable $x$, such that

$$f(x) - f(x^*) \leq \epsilon$$

for any given user-specified precision level $\epsilon > 0$. In this paper, we consider this selection problem in a large decision space with high dimension. Instead of treating each decision variable as an alternative that is independent of all others, we explore how the structure of a selection problem can help the selection procedure. We consider selection problems that have a discrete convex structure on the objective function.

**Assumption 1.** The objective function $f(x)$ is a convex function on the discrete set $\mathcal{X}$.

We note that the convexity of a function on a discrete set is not equivalent to that the function can be extended to a continuous convex function. For the exact definition of convexity of functions supported on a discrete set, we describe in details in Section 2.3.

Because $f$ does not have a closed-form representation and has to be evaluated by simulation, we take the view that no further structure information is available in addition to the convex structure. For instance, for a real-world model, $f$ may have a very flat landscape around the minimum, which may not be known a priori. In this case, there may be a number of decision variables that render objective value that is at most $\epsilon$ apart from the optimal. This also motivates our goal to select a good decision variable instead of the best, because too much computational resource may be needed to identify exactly the best, when the landscape around the minimum is flat. Therefore, our general goal is to develop simulation algorithms that are expected to robustly work for any convex model without knowing further specific structure.
Because the precision level $\epsilon$ cannot be delivered almost surely with finite computational budget for simulation, we consider a selection optimality guarantee called *Probability of Good Selection*; see Eckman and Henderson (2018a,b), Hong et al. (2020).

- **Probability of good selection (PGS).** The solution $x$ returned by an algorithm has objective value at most $\epsilon$ larger than the optimal objective value with probability at least $1 - \delta$.

This PGS guarantee is also called the probably approximately correct selection (PAC) guarantee in the literature (Even-Dar et al. 2002, Kaufmann et al. 2016, Ma and Henderson 2017). While our focus is to design algorithms that satisfy the PGS optimality guarantee, we also consider the optimality guarantee of *Probability of Correct Selection with Indifference Zone* as a comparison.

- **Probability of correct selection with indifference zone (PCS-IZ).** The problem is assumed to have a unique solution that renders the optimal objective value. The optimal value is assumed to be at least $c > 0$ smaller than other objective values. The gap width $c$ is called the **indifference zone parameter** in Bechhofer (1954). The PCS-IZ guarantee requires that the solution returned by an algorithm is the optimal solution with probability at least $1 - \delta$.

By choosing $\epsilon < c$, algorithms satisfying the PGS guarantee can be directly applied to satisfy the PCS-IZ guarantee. On the other hand, counterexamples in Eckman and Henderson (2018a) show that algorithms satisfying the PCS-IZ guarantee may fail to satisfy the PGS guarantee. This phenomenon is further explained from the hypothesis-testing perspective in Hong et al. (2020). The failing probability $\delta$ in either PGS or PCS-IZ is typically chosen to be very small to ensure a high probability result. Hence, we assume in the following of this paper that $\delta$ is small enough.

**Assumption 2.** *The failing probability $\delta$ is sufficiently small.*

To facilitate the construction of simulation algorithms that can deliver PGS guarantee for general convex problems, we specify the composition of simulation algorithms in the next subsection. In addition, we assume that the probability distribution for the simulation output $F(x, \xi_x)$ is sub-Gaussian.
Assumption 3. The distribution of $F(x, \xi_x)$ is sub-Gaussian with known parameter $\sigma^2$ for any $x \in \mathcal{X}$.

One special case for Assumption 3 is that the probability distribution for a system labeled by $x$ is Gaussian with variance $\sigma_x^2$, for which an upper bound $\sigma^2 \geq \max_{x \in \mathcal{X}} \sigma_x^2$ is known. The specific value of variance $\sigma_x^2$ for each system can be unknown. Another special case for Assumption 3 is that the random quantity $F(x, \xi_x)$ is bounded.

2.1. Simulation Algorithms

In this subsection, we define the different specifics of simulation algorithms. We hope to design simulation algorithms that can deliver certain optimality guarantee, say, PGS, for any convex model without knowing further structure. A broad range of sequential simulation optimization algorithms consist of three parts.

- The **sampling rule** determines which system to simulate next, based on the history of simulation observations up to current time.

- The **stopping rule** controls the end of the simulation phase and is a stopping time according to the filtration up to current time. We assume that the stopping time is finite almost surely.

- The **recommendation rule** selects the system that satisfies the optimality guarantee based on the history of simulation observations.

The **model** of problem (1) consists of the decision set $\mathcal{X}$, the space of randomness $(\mathcal{Y}, \mathcal{B}_\mathcal{Y})$ and the function $F(\cdot, \cdot)$. We define the set of all models such that the objective function $f(\cdot)$ is convex on the discrete set $\mathcal{X}$ as $\mathcal{MC}(\mathcal{X})$, or simply $\mathcal{MC}$. Next, we define the class of simulation algorithms that can deliver solutions satisfying certain optimality guarantee for a given set of models.

**Definition 1.** Suppose the optimality guarantee $\mathcal{O}$ and the set of models $\mathcal{M}$ is given. A simulation algorithm is called an $(\mathcal{O}, \mathcal{M})$-algorithm, if for any model $M \in \mathcal{M}$, the algorithm returns a solution to $M$ that satisfies the optimality guarantee $\mathcal{O}$.

Using this definition, a $(\text{PGS}, \mathcal{MC})$-algorithm is one that guarantees the finding of a solution that satisfies the PGS guarantee for any convex model without knowing further structure.
2.2. Simulation Costs

In the development of simulation algorithms that satisfy certain optimality guarantee, especially for large-scale problems, the performance of different algorithms can be compared based on their computational costs to achieve the same optimality guarantee. We take the view that the simulation cost of generating replications of \( F(x, \xi_x) \) is the dominant contributor to the computational cost associated with a simulation algorithm. See also Luo et al. (2015), Ni et al. (2017), and Ma and Henderson (2019). Therefore, we quantify the computational cost as the total number of evaluations of \( F(x, \xi_x) \) at different \( x \). In some simulation problems but not all, we may also have access to noisy and possibly biased estimates of \( f(\cdot) \) near point \( x \) along with an evaluation of \( F(x, \xi_x) \). The simulation cost in this case is discussed in Section 6. For all simulation algorithms proposed in this paper, we analyze and provide upper bounds on the expected simulation cost to achieve a certain optimality guarantee. Note that these upper bounds do not rely on the specific structure of the selection problem in addition to convexity. The benefits of this simulation cost analysis are three folds. First, the expected simulation cost serves as a measurement to compare different algorithms. Second, the upper bounds on expected simulation costs provide insights on how the computational cost depends on the scale and dimension of the problem. On the other hand, understanding the expected simulation costs can provide information to facilitate the setup of parallel procedures for large-scale problems.

Now, we define the expected simulation cost for a given set of models \( \mathcal{M} \) and given optimality guarantee \( \mathcal{O} \).

**Definition 2.** Given the optimality guarantee \( \mathcal{O} \) and a set of models \( \mathcal{M} \), the **expected simulation cost** is defined as

\[
T(\mathcal{O}, \mathcal{M}) := \inf_{\mathbf{A} \text{ is } (\mathcal{O}, \mathcal{M})} \sup_{M \in \mathcal{M}} \mathbb{E}[^{\mathcal{O}}] \tau, \]

where \( \tau \) is the stopping time of the algorithm, which is also the number of simulation evaluations of \( F(\cdot, \cdot) \).
The notion of simulation cost in this paper is largely focused on

\[ T(\epsilon, \delta, \mathcal{MC}) := T((\epsilon, \delta)-\text{PGS}, \mathcal{MC}) \]
\[ T(\delta, \mathcal{MC}_c) := T((c, \delta)-\text{PCS-IZ}, \mathcal{MC}_c). \]

Note that the \((\epsilon, \delta)-\text{PGS}\) refers to the PGS optimality guarantee with user-specified precision level \(\epsilon > 0\) and confidence level \(1 - \delta\). The notion \((c, \delta)-\text{PCS-IZ}\) refers to the PCS-IZ optimality guarantee with confidence level \(1 - \delta\) and IZ parameter \(c\). The class of models \(\mathcal{MC}\) include all convex models while \(\mathcal{MC}_c\) include all convex models with IZ parameter \(c\). In addition, we mention that all upper bounds derived in this paper are actually almost sure bounds of the simulation cost, while lower bounds only hold in expectation.

To better present the dependence of expected simulation cost on the scale and dimension of the problem, in this work, we assume that \(N_1 = N_2 = \cdots = N_d\).

**Assumption 4.** *The feasible set of decision variables is \(X = [N]^d\), where \(N \geq 2\) and \(d \geq 1\).*

In large-scale simulation problems, either \(N\), or \(d\), or both \(N\) and \(d\) can be large. With Assumption 4 in hand, we will present the dependence of the expected simulation on \(N\) and \(d\) when at least one of them is large. We note that the results under Assumption 4 can be naturally extended to the case when each dimension has different number of feasible systems, i.e., \(X = [N_1] \times [N_2] \times \cdots \times [N_d]\).

Furthermore, if the objective function \(f\) is defined on the cube \([N_1] \times [N_2] \times \cdots \times [N_d]\) while the feasible set \(X\) is a convex set in the cube, the simulation algorithms proposed in this paper can be extended with minor modifications.

### 2.3. Discrete Convex Functions in Multi-dimensional Space

In contrast to the continuous case, the discrete convexity has various different definitions, e.g., convex extensible functions and submodular functions. Although these concepts coincide for the one-dimensional case, they have essential differences in the multi-dimensional case. In this work, we consider \(L^3\)-convex functions (Murota 2003), which is defined by the mid-point convexity for discrete variables. Considerably many discrete simulation optimization problems have the \(L^3\)-convex
structure. For example, the expected customer waiting time in a multi-server queueing network is proved to be a separated convex function \cite{Altman2003, Wolfl2002} and therefore is $L^3$-convex. In addition, the dissatisfaction function of bike-sharing system is shown to be multi-modular in \cite{Freund2017}, which is $L^2$-convex under a linear transformation. More examples of $L^3$-convex functions are given in \cite{Murota2003}. On the other hand, the minimization of a $L^3$-convex function is equivalent to the minimization of its linear interpolation, which is continuous and convex. Combining with the closed-form subgradient, $L^3$-convex functions provide a good framework for studying discrete convex simulation optimization problems.

Before we give the definition of $L^3$-convexity, we first show that it is not suitable to define discrete convex functions just as functions that have convex extension. The main problem of this definition based on extension is that the local optimality may not be equivalent to the global optimality, which is one of the important properties used in convex optimization. Without this property, algorithms may stick at spurious local minima and fail to satisfy the optimality guarantee. We give an example to illustrate the failure.

**Example 1.** We consider the case when $N = 4$ and $d = 2$. The objective function is given as

$$f(x, y) := 4|2x + y - 8| + |x - 2y + 6|.$$ 

The function $f(x, y)$ is a convex function on the set $[1, 4]^2$ and the unique global minimizer is $(2,4)$. When restricted to the integer lattice $\{1,2,3,4\}^2$, the global minimizer is still $(2,4)$. We consider the point $(3,2)$ with objective value $f(3,2) = 5$. In the local neighborhood $\{2,3,4\} \times \{1,2,3\}$, the objective values are

$$f(2,1) = 18, \ f(3,1) = 11, \ f(4,1) = 12, \ f(2,2) = 12,$$

$$f(4,2) = 14, \ f(2,3) = 6, \ f(3,3) = 7, \ f(4,3) = 16.$$ 

Thus, the point $(3,2)$ is a spurious local minimizer of the discrete function. This shows that local optimality can not imply global optimality.
On the other hand, the $L^\natural$-convexity ensures that local optimality implies global optimality. In Murota (2003), $L^\natural$-convex functions are introduced as an extension to submodular functions and are proved to have the above property. Similar to the continuous case, $L^\natural$-convex functions can be characterized by the discrete midpoint convexity property. The exact definition is given by

**Definition 3.** A function $f(x) : \mathcal{X} \mapsto \mathbb{R}$ is called a $L^\natural$-convex function, if the discrete midpoint convexity holds:

$$f(x) + f(y) \geq f(\lfloor (x+y)/2 \rfloor) + f(\lceil (x+y)/2 \rceil) \quad \forall x, y \in \mathcal{X}.$$ 

The set of models such that $f(x)$ is $L^\natural$-convex on $\mathcal{X}$ is denoted as $MC$. The set of models such that $f(x)$ is $L^\natural$-convex with indifference zone parameter $c$ is denoted as $MC_c$.

**Remark 1.** In general, the definition of $L^\natural$-convexity also requires the feasible set $\mathcal{X}$ to be a $L^\natural$-convex set, namely, the indicator function of $\mathcal{X}$ should be $L^\natural$-convex on $\mathbb{Z}^d$. In our case, the feasible set $\mathcal{X} = [N]^d$ is a $L^\natural$-convex set. Hence, we only need the discrete midpoint convexity property to define $L^\natural$-convex functions on $\mathcal{X}$.

It is proved in Murota (2003) that $L^\natural$-convex functions share properties of both ordinary convex functions and submodular functions. In the following lemma, we list several properties of $L^\natural$-convex functions.

**Lemma 1.** Suppose the function $f(x) : \mathcal{X} \mapsto \mathbb{R}$ is $L^\natural$-convex. The following properties hold.

- There exists a convex function $\tilde{f}(x)$ on $[1, N]^d$ such that $\tilde{f}(x) = f(x)$ for $x \in \mathcal{X}$.

- Local optimality is equivalent to global optimality:

$$f(x) \leq f(y) \quad \forall y \in \mathcal{X} \iff f(x) \leq f(y) \quad \forall y \in \mathcal{X} \quad \text{s.t.} \quad \|y - x\|_\infty = 1.$$ 

- Translation submodularity holds:

$$f(x) + f(y) \geq f((x - \alpha 1) \lor y) + f(x \land (y + \alpha 1)) \quad \forall x, y \in \mathcal{X}, \alpha \in \mathbb{N} \text{ s.t. } (x - \alpha 1) \lor y, x \land (y + \alpha 1) \in \mathcal{X}.$$
The $L^\natural$-convexity can be viewed as a combination of submodularity and integral convexity (Murota 2003, Theorem 7.20). Intuitively, the submodularity ensures the existence of a piecewise linear convex interpolation in the local neighborhood of each point, while the integral convexity ensures that the piecewise linear convex interpolations can be pieced together to form a convex function on $[1, N]^d$. In addition, we can calculate a subgradient of the convex extension with $O(d)$ function value evaluations. Hence, $L^\natural$-convex functions provides a good framework for extending continuous convex optimization theory to the discrete case.

3. Simulation Algorithms and Expected Simulation Costs for a Special Case

In this section and the following section, we propose simulation algorithms that achieve the PGS guarantee for any simulation optimization problem with $L^\natural$-convex objective function. We prove upper bounds on the expected simulation costs. The decision space is considered as $\mathcal{X} = [N]^d$. In this section, we start with a special case when $N = 2$, so that the decision space is $\{0,1\}^d$ for a large $d$. We defer the discussions for general $N$ and $d$ to Section 4. We have in mind cases where the dimension $d$ is large. Each replication of simulation can only output a noisy evaluation of the function value at a given discrete decision variable. The simulator may have a general complex and discontinuous structure that no unbiased gradient estimator is available within the replication of simulation. For scenarios when a single replication of simulation can also generate gradient information at very low costs, we propose and analyze simulation algorithms in Section 6.

The general idea of designing simulation algorithm in the multi-dimensional case is to construct subgradients of the convex extension with $O(d)$ function value evaluations on the neighbor of a decision variable. Hence, the stochastic subgradient descent (SSGD) method can be used to solve problem (11). Compared with the bi-section method and general cutting plane methods, gradient-based methods have two advantages in our case. First, as pseudo-polynomial algorithms, gradient-based methods usually have lighter dependence on the problem dimension $d$ compared to strongly polynomial or weakly polynomial algorithms. For example, the deterministic integer-valued submodular function minimization (SFM) problem can be solved with $\tilde{O}(d), \tilde{O}(d^2), \tilde{O}(d^3)$ function value...
evaluations using pseudo-polynomial (Axelrod et al. 2020), weakly polynomial and strongly polynomial (Lee et al. 2015) algorithms, respectively. Usually, gradient-based methods have extra polynomial dependence on the Lipschitz constant of the objective function, in exchange for the reduced dependence on \( d \). However, the Lipschitz constant of a large group of problems may be estimated a priori. Moreover, we can design algorithms whose expected simulation cost does not critically rely on the Lipschitz constant, in the sense that the Lipschitz constant only appears in a smaller order term in the expected simulation cost. Hence, gradient-based methods are preferred for high-dimensional problems. On the other hand, ordinary cutting plane methods are not robust to noise and problem-specific stabilization techniques should be designed for stochastic problems (Sen and Higle 2001), or complicated robust scheme should be constructed (Nemirovsky and Yudin 1983, Agarwal et al. 2011). Considering these two advantages of gradient-based methods, we focus on the SSGD method in designing our simulation algorithms and make the assumption that the \( \ell_\infty \)-Lipschitz constant can be estimated a priori.

**Assumption 5.** The \( \ell_\infty \)-Lipschitz constant of \( f(x) \) is \( L \). Namely, we have

\[
|f(x) - f(y)| \leq L \quad \forall x, y \in \mathcal{X}, \quad \text{s.t.} \quad \|x - y\|_\infty \leq 1.
\]

We remark that this constant \( L \), in the general decision making contexts, reflects the impact on the objective function by a small change in one coordinate the high-dimensional decision variable. For example, in bike-sharing applications, this \( L \) may reflect the impact of allocating one more bike to a station. Whether the objective function being revenue or number of dissatisfied customers, the upper bound on the impact of allocating one more bike can be quantified.

When \( N = 2 \) and the decision space is \( \mathcal{X} = \{0, 1\}^d \), \( L^3 \)-convex functions are equivalent to submodular functions and therefore problem (11) is equivalent to the stochastic submodular function minimization (stochastic SFM) problem. To prepare the design of simulation algorithms, we first define the Lovász extension of submodular functions and give an explicit subgradient of the Lovász extension at each point.
**Definition 4.** Suppose function $f(x) : \{0,1\}^d \rightarrow \mathbb{R}$ is a submodular function. For any $x \in [0,1]^d$, we say a permutation $\alpha_x : [d] \rightarrow [d]$ is a **consistent permutation** of $x$, if

$$x_{\alpha_x(1)} \geq x_{\alpha_x(2)} \geq \cdots \geq x_{\alpha_x(d)}.$$

For each $i \in \{0,1,\ldots,d\}$, the **$i$-th neighbouring points** of $x$ is defined as

$$S^{x,i} := \sum_{j=1}^{i} e_{\alpha_x(j)} \in \mathcal{X},$$

where vector $e_k$ is the $k$-th unit vector of $\mathbb{R}^d$. We define the **Lovász extension** $\tilde{f}(x) : [0,1]^d \rightarrow \mathbb{R}$ as

$$\tilde{f}(x) := f(S^{x,0}) + \sum_{i=1}^{d} \left[ f(S^{x,i}) - f(S^{x,i-1}) \right] x_{\alpha_x(i)}.$$  \hspace{1cm} (2)

We note that the value of the Lovász extension does not rely on the consistent permutation we choose. We list several well-known properties of the Lovász extension and refer their proofs to Lovász (1983), Fujishige (2005). We note that the subgradient at point $x \in [1,N]^d$ is defined as the set

$$\partial \tilde{f}(x) = \left\{ g \in \mathbb{R}^d : \langle g, x - y \rangle \geq \tilde{f}(x) - \tilde{f}(y), \forall y \in [1,N]^d \right\}.$$

**Lemma 2.** Suppose Assumptions 1-5 hold. Then, the following properties of $\tilde{f}(x)$ hold.

(i) For any $x \in \mathcal{X}$, it holds $\tilde{f}(x) = f(x)$.

(ii) The minimizers of $\tilde{f}(x)$ satisfy $\operatorname{arg \, min}_{x \in [0,1]^d} \tilde{f}(x) = \operatorname{arg \, min}_{x \in \mathcal{X}} f(x)$.

(iii) Function $\tilde{f}(x)$ is a convex function on $[0,1]^d$.

(iv) A subgradient $g \in \partial \tilde{f}(x)$ is given by

$$g_{\alpha_x(i)} := f(S^{x,i}) - f(S^{x,i-1}) \quad \forall i \in [d].$$  \hspace{1cm} (3)

(v) Subgradients of $\tilde{f}(x)$ satisfy

$$\|g\|_1 \leq 3L/2 \quad \forall g \in \partial \tilde{f}(x), \ x \in [0,1]^d.$$
To apply the SSGD method to design simulation algorithms for problem (1), we need to resolve the following two questions:

- How to design an unbiased subgradient estimator?
- How to round an approximate solution in \([0,1]^d\) to an approximate solution in \(X = \{0, 1\}^d\)?

For the first question, we consider the subgradient estimator at point \(x\) as

\[
\hat{g}_{\alpha x(i)} := F(S^x,i, \xi_i) - F(S^x,i-1, \xi_{i-1}) \quad \forall i \in [d].
\]

(4)

By definition, we know components of \(\hat{g}\) are mutually independent and the simulation cost of each \(\hat{g}\) is \(2d\). Using the subgradient defined in (3), we have

\[
E[\hat{g}_{\alpha x(i)}] = E[F(S^x,i, \xi_i) - F(S^x,i-1, \xi_{i-1})] = f(S^x,i) - f(S^x,i-1) = g_{\alpha x(i)} \quad \forall i \in [d],
\]

which means that \(\hat{g}\) is an unbiased estimator of \(g\). Next, we consider the second question. We define the relaxed problem as

\[
f^* := \min_{x \in [0,1]^d} \tilde{f}(x).
\]

(5)

Properties (i) and (ii) of Lemma 2 imply that the original problem (1) is equivalent to the relaxed problem (5). In the deterministic case, suppose we already have an \(\epsilon\)-optimal solution to problem (5), i.e., a point \(\bar{x}\) in \([0,1]^d\) such that \(\tilde{f}(\bar{x}) \leq f^* + \epsilon\). Then, we rewrite the Lovász extension in (2) as

\[
\tilde{f}(\bar{x}) = [1 - \bar{x}_{\alpha z(1)}] f(S^{\bar{x},0}) + \sum_{i=1}^{d-1} [\bar{x}_{\alpha z(i)} - \bar{x}_{\alpha z(i+1)}] f(S^{\bar{x},i}) + \bar{x}_{\alpha z(d)} f(S^{\bar{x},d}),
\]

(6)

which is a convex combination of \(f(S^{\bar{x},0}), \ldots, f(S^{\bar{x},d})\). Hence, there exists an \(\epsilon\)-optimal solution among the neighboring points of \(\bar{x}\). This means that we can solve a sub-problem with \(d+1\) points to get the \(\epsilon\)-optimal solution among neighboring points. For the stochastic case, a similar rounding process can be designed and we give the pseudo-code in Algorithm 1.

**Algorithm 1** Rounding process to a feasible solution
**Input:** Model $\mathcal{X}, \mathcal{B}_x, F(x, \xi_x)$, optimality guarantee parameters $\epsilon, \delta, (\epsilon/2, \delta/2)$-PGS solution $\bar{x}$ to problem (5).

**Output:** An $(\epsilon, \delta)$-PGS solution $x^*$ to problem (1).

1: Compute a consistent permutation of $\bar{x}$, denoted as $\alpha$.

2: Compute the neighbouring points of $\bar{x}$, denoted as $S^0, \ldots, S^d$.

3: Simulate $F(S^0, \xi_0), \ldots, F(S^d, \xi_d)$ until the $1 - \delta/4$ confidence width is smaller than $\epsilon/4$.

4: Return the point $x^*$ with minimal empirical mean.

The following theorem proves the correctness and estimates the simulation cost of Algorithm 1.

Note that all the upper bound results on simulation costs in this paper are proved to hold both almost surely and in expectation. We do not differentiate the use of simulation costs and expected simulation costs in upper bound results.

**Theorem 1.** Suppose Assumptions 1-5 hold. The solution returned by Algorithm 1 satisfies the $(\epsilon, \delta)$-PGS guarantee. The simulation cost of Algorithm 1 is at most

$$O \left[ \frac{d\epsilon^2}{\delta} \log \left( \frac{1}{\delta} \right) + d \right] = \tilde{O} \left[ \frac{d\epsilon^2}{\delta} \log \left( \frac{1}{\delta} \right) \right].$$

**Proof of Theorem 1.** The proof of Theorem 1 is given in EC.1.1. □

The rounding process for the $(c, \delta)$-PCS-IZ guarantee follows by choosing $\epsilon = c/2$. After resolving these two problems, we can first use the SSGD method to find an approximate solution to problem (5) and then round the solution to get an approximate solution to problem (1). Hence, the focus of the remainder of this section is to provide upper bounds of simulation cost to the SSGD method.

The main difficulty of giving sharp upper bounds lies in the fact that the Lovász extension is neither smooth nor strongly-convex. This property of the Lovász extension prohibits the application of Nesterov acceleration and common variance reduction techniques.

Now, we propose the projected and truncated SSGD method for the $(\epsilon, \delta)$-PGS guarantee. The orthogonal projection onto the feasible set, which is defined as

$$\mathcal{P}(x) := (x \land 1) \lor 0 \quad \forall x \in \mathbb{R}^d,$$
is applied after each iteration to ensure the feasibility of iteration point. In addition to the projection, componentwise truncation of stochastic subgradient is critical in reducing expected simulation costs. The truncation operator with threshold $M > 0$ is defined as

$$T_M(g) := (g \wedge M1) \vee (-M1) \forall g \in \mathbb{R}^d.$$ 

The pseudo-code of projected and truncated SSGD method is listed in Algorithm 2.

**Algorithm 2** Projected and truncated SSGD method for PGS guarantee

**Input:** Model $\mathcal{X}, B_x, F(x, \xi_x)$, optimality guarantee parameters $\epsilon, \delta$, number of iterations $T$, step size $\eta$, truncation threshold $M$.

**Output:** An $(\epsilon, \delta)$-PGS solution $x^*$ to problem (1).

1: Choose the initial point $x^0 \leftarrow (N/2, \ldots, N/2)^T$.
2: for $t = 0, \ldots, T - 1$ do
3: Generate a stochastic subgradient $\hat{g}^t$ at $x^t$.
4: Truncate the stochastic subgradient $\tilde{g}^t \leftarrow T_M(\hat{g}^t)$.
5: Update $x^{t+1} \leftarrow P(x^t - \eta\tilde{g}^t)$.
6: end for
7: Compute the averaging point $\bar{x} \leftarrow (\sum_{t=0}^{T-1} x^t) / T$.
8: Round $\bar{x}$ to an integral point by Algorithm 1.

The analysis of Algorithm 2 fits into the classical convex optimization framework. The following Azuma’s inequality for martingales with sub-Gaussian tails plays as a major role for deriving high-probability bounds.

**Lemma 3** (Azuma’s inequality for sub-Gaussian tails (Shamir 2011)). Let $X_0, \ldots, X_{T-1}$ be a martingale difference sequence. Suppose there exist constants $b_1 \geq 1, b_2 > 0$ such that, for any $t \in \{0, \ldots, T-1\}$,

$$P(|X_t| \geq a \mid X_1, \ldots, X_{t-1}) \leq 2b_1 \exp(-b_2a^2) \forall a \geq 0.$$ 

(7)
Then for any $\delta > 0$, it holds with probability at least $1 - \delta$ that

$$\frac{1}{T} \sum_{t=0}^{T-1} X_t \leq \sqrt{\frac{28b_1}{b_2T \log(\frac{1}{\delta})}}.$$ 

With a suitable choice of the step size, the truncation threshold and the number of iterations, Algorithm 2 returns an $(\epsilon, \delta)$-PGS solution and the expected simulation cost has $O(d^2)$ dependence on the dimension.

**Theorem 2.** Suppose Assumptions 1-5 hold and the subgradient estimator in (4) is used. If we choose

$$T = \tilde{\Theta} \left[ \frac{d^2}{\epsilon^2} \log\left(\frac{1}{\delta}\right) \right], \quad M = \tilde{\Theta} \left[ \sqrt{\log\left(\frac{d}{\epsilon}\right)} \right], \quad \eta = \frac{1}{M \sqrt{d}}$$

then Algorithm 2 returns an $(\epsilon, \delta)$-PGS solution. Furthermore, we have

$$T(\epsilon, \delta, \mathcal{M}C) = \tilde{O} \left[ \frac{d^2}{\epsilon^2} \log\left(\frac{1}{\delta}\right) + d^3 \log\left(\frac{d^2}{\epsilon^3}\right) + \frac{d^3L^2}{\epsilon^2} \right] = \tilde{O} \left[ \frac{d^2}{\epsilon^2} \log\left(\frac{1}{\delta}\right) \right].$$

**Proof of Theorem 2.** The proof of Theorem 2 is given in EC.1.2. 

Although independent of $\delta$, we note that the last two terms in the expected simulation cost may be comparable to the first term when $\delta$ is not that small. We can prove that, without the truncation step ($M = \infty$), the expected simulation becomes

$$\tilde{O} \left[ \frac{d^3}{\epsilon^2} \log\left(\frac{1}{\delta}\right) \right].$$

Hence, the truncation of stochastic subgradient is necessary for reducing the asymptotic expected simulation cost. By choosing $\epsilon = c/2$, Algorithm 2 returns a $(c, \delta)$-PCS-IZ solution and the expected simulation cost for the PCS-IZ guarantee is

$$T(\delta, \mathcal{M}C_c) = \tilde{O} \left[ \frac{d^2}{c^2} \log\left(\frac{1}{\delta}\right) \right].$$

We note that the expected simulation cost for both guarantees does not critically depend on the Lipschitz constant $L$. As an alternative to estimator (4), we may consider generating a stochastic subgradient by randomly choosing a subset of components and only estimating the chosen components of subgradients. However, using this estimator, we can not achieve better simulation cost
and the expected simulation cost may be critically dependent on $L$. To be more concrete, given $k \in [d]$, we can use the following procedure to generate a stochastic subgradient with $k$ nonzero components:

1. Select a $k$-element set $I \subset [d]$ uniformly at random.

2. Compute

\[
\hat{g}_{\alpha_x(i)} := \frac{d}{k} \left[ F \left( S^{x,i}, \xi^1_i \right) - F \left( S^{x,i-1}, \xi^2_{i-1} \right) \right] \quad \forall i \in [d] \text{ s.t. } \alpha_x(i) \in I.
\]  

(8)

We can see that estimator (8) is a special case of estimator (8) when $k = d$. Since each component $\alpha_x(i)$ has probability $k/d$ to be chosen in the set $I$, we have

\[
\mathbb{E} \left[ \hat{g}_{\alpha_x(i)} \right] = \frac{k}{d} \mathbb{E} \left[ \alpha_x(i) \mid \alpha_x(i) \in I \right] = \mathbb{E} \left[ F \left( S^{x,i}, \xi^1_i \right) - F \left( S^{x,i-1}, \xi^2_{i-1} \right) \right] = f \left( S^{x,i} \right) - f \left( S^{x,i-1} \right) = g_{\alpha_x(i)},
\]

which implies that estimator (8) is also unbiased. We can estimate the expected simulation cost using estimator (8) in the same way as Theorem 2. Here we intuitively show that the expected simulation cost is not improved and may depend on the Lipschitz constant when $k < d$. The proof of Theorem 2 implies that the expected simulation cost of Algorithm 2 is approximately

\[
\tilde{O} \left[ k \cdot \mathbb{E} \left[ \| \hat{g} - g \|_1 \right]^2 \cdot \frac{1}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].
\]

Suppose set $I$ is selected when generating $\hat{g}$. Then, we have

\[
\mathbb{E} \left[ \| \hat{g}_I - g_I \|_1 \right] = \mathbb{E} \left[ \| \hat{g}_I - g_I \|_1 \right] + \mathbb{E} \left[ \| \hat{g}_I - g_I \|_1 \right] = \mathbb{E} \left[ \| \hat{g}_I - g_I \|_1 \right] + \mathbb{E} \left[ \| g_I \|_1 \right],
\]

(9)

where we define $(x_I)_i := x_i$ for $i \in I$ and $(x_I)_i := 0$ otherwise. By property (v) in Lemma 2, we have $\|g\|_1 \leq 3L/2$ and therefore

\[
\mathbb{E} \left[ \| g_I \|_1 \right] = O(L), \quad \mathbb{E} \left[ \| g_I \|_1 \right] = O \left[ (d - k)L \right].
\]

By the definition of estimator (8), we know that

\[
\| \hat{g}_I - \mathbb{E} \left[ \hat{g}_I \right] \|_1 = \| \hat{g}_I - d/k \cdot g_I \|_1
\]
is the sum of \( k \) independent sub-Gaussian random variables with parameter \( \sigma^2 \) scaled by \( d/k \).

Hence, random variable \( \| \hat{g}_I - \mathbb{E}[\hat{g}_I] \|_1 \) is sub-Gaussian with parameter \( d^2/k \cdot \sigma^2 \) and

\[
\mathbb{E}[\| \hat{g}_I - g_I \|_1] = O\left( \sqrt{\frac{d^2}{k} \cdot \sigma} \right).
\]

Substituting the above estimates into (9), we get

\[
\mathbb{E}[\| \hat{g}_i - g_i \|_1] = \mathbb{E}[\| \hat{g}_I - g_I \|_1] + \mathbb{E}[\| g_J \|_1] = \mathbb{E}\left[ \left\| \hat{g}_I - \frac{d}{k} \cdot g_I \right\|_1 + \left( \frac{d}{k} - 1 \right) \cdot g_I \right] + \mathbb{E}[\| g_J \|_1]
\approx \mathbb{E}\left[ \left\| \hat{g}_I - \frac{d}{k} \cdot g_I \right\|_1 \right] + \left( \frac{d}{k} - 1 \right) \cdot \mathbb{E}[\| g_I \|_1] + \mathbb{E}[\| g_J \|_1]
\approx O\left( \sqrt{\frac{d^2}{k} \cdot \sigma + (d - k) L} \right).
\]

This implies that the expected simulation cost using estimator (8) is approximately

\[
\tilde{O}\left[ k \cdot \left( \frac{d^2}{k} \cdot \sigma^2 + (d - k)^2 L^2 \right) \cdot \frac{1}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right] = \tilde{O}\left[ \frac{d^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) + \frac{(d - k)^2 L^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].
\]

We can see that the first term of the expected simulation cost is the same as Theorem 2 and there is an extra term depending on \( L \) if we choose \( k < d \). Therefore, estimator (8) is not expected to be better than estimator (4) when \( k < d \).

Before finishing the discussion of stochastic SFM problem, we consider a special case when the stochastic subgradient is assumed to have a bounded norm. In the field of stochastic optimization, this assumption is common when analyzing the high-probability convergence of stochastic subgradient methods (Hazan and Kale 2011, Xu et al. 2016). In this work, we also consider the case when the following assumption holds and estimate the expected simulation cost.

**Assumption 6.** There exist a constant \( G \) and an unbiased subgradient estimator \( \hat{g} \) such that

\[
P[\| \hat{g} \|_1 \leq G] = 1.
\]

Moreover, the simulation cost of generating each \( \hat{g} \) is at most \( \beta \) simulations.

We note that \( G \) and \( \beta \) may depend on \( d \) and \( N \). We first give two examples where Assumption 6 holds.
Example 2. We consider the case when the randomness of each system shares the same measure space, i.e., there exists a measure space \((Z, \mathcal{B}_Z)\) such that \(\xi_x\) can be any element in the measure space for all \(x \in \mathcal{X}\). Moreover, for any fixed \(\xi \in \mathcal{B}\), the function \(F(\cdot, \xi)\) is also \(L^2\)-convex (or submodular when \(N = 2\)) and has \(\ell_\infty\)-Lipschitz constant \(\tilde{L}\). Then, we consider the subgradient estimator

\[
\hat{g}_{\alpha x(i)} := F(S^{x,i}, \xi) - F(S^{x,i-1}, \xi) \quad \forall i \in [d].
\]

The simulation cost of estimator (10) is \(d + 1\). In addition, property (v) of Lemma 2 gives

\[
\|\hat{g}\|_1 \leq \frac{3\tilde{L}}{2}.
\]

Therefore, in this situation, the Assumption 6 holds with \(G = \frac{3\tilde{L}}{2}\) and \(\beta = d + 1\).

When the distribution at each system is the Bernoulli, we show that Assumption 6 also holds.

Example 3. We consider the case when the distribution at each point \(x \in \mathcal{X}\) is Bernoulli, namely, we have

\[
P[F(x, \xi_x) = 1] = 1 - P[F(x, \xi_x) = 0] = f(x) \in [0, 1] \quad \forall x \in \mathcal{X}.
\]

We note that the Bernoulli distribution is a special case of sub-Gaussian distributions. In this case, the \(\ell_\infty\)-Lipschitz constant is 1 and property (v) in Lemma 2 gives \(\|g\|_1 \leq \frac{3}{2}\) for any subgradient \(g\). We consider the subgradient estimator (8). At point \(x\), if set \(I\) is chosen, then we know that

\[
\|\hat{g}\|_1 = \frac{d}{k} \cdot \sum_{i \in I} \left| F(S^{x,i}, \xi^1) - F(S^{x,i-1}, \xi^2) \right| \leq \frac{d}{k} \cdot |I| = d.
\]

Hence, Assumption 6 holds with \(G = \frac{d}{k}\) and \(\beta = 2k\).

Next, we estimate the expected simulation cost of Algorithm 2 under Assumption 6. Since the stochastic gradient is bounded, we apply the Azuma’s inequality for martingale difference sequences with bounded tails.

**Lemma 4** (Azuma’s inequality with bounded tails). Let \(X_0, \ldots, X_{T-1}\) be a martingale difference sequence. Suppose there exists a constant \(b\) such that for any \(t \in \{0, \ldots, T-1\},\)

\[
P(|X_t| \leq b) = 1.
\]
Then for any $\delta > 0$, it holds with probability at least $1 - \delta$ that
\[
\frac{1}{T} \sum_{t=0}^{T-1} X_t \leq b \sqrt{\frac{2}{T} \log \left( \frac{1}{\delta} \right)}.
\] (11)

Also, since the stochastic subgradient is bounded, the truncation step is unnecessary in Algorithm 2. The simulation cost of Algorithm 2 is estimated in the following theorem. The proof is similar to Lemma 10 in Hazan and Kale (2011) and, since the feasible set is the cube $[0,1]^d$, we use $\ell_\infty$-norm instead of $\ell_2$-norm to bound distances between points.

**Theorem 3.** Suppose Assumptions 1-6 hold. If we skip the truncation step in Algorithm 2 (i.e., set $M = \infty$) and choose
\[
T = \tilde{\Theta} \left[ \frac{(L+G)^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right], \quad \eta = \sqrt{\frac{d}{TG^2}},
\]
then Algorithm 2 returns an $(\epsilon, \delta)$-PGS solution. Furthermore, we have
\[
T(\epsilon, \delta, MC) = O \left( \frac{\beta(L+G)^2 + d}{\epsilon^2} \log \left( \frac{1}{\delta} \right) + \frac{d^2G^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right).
\]

**Proof of Theorem 3.** The proof of Theorem 3 is given in EC.1.3. \hfill \square

In the case of Example 2, we have $\beta = d + 1, G = 3\tilde{L}/2$ and then the asymptotic simulation cost of Algorithm 2 is at most
\[
\tilde{O} \left[ \frac{d(L+\tilde{L})^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].
\]
If both Lipschitz constants are independent of $d$ and $N$, the asymptotic simulation cost becomes
\[
\tilde{O} \left[ \frac{d}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right],
\]
which is $O(d)$ better than the general case without Assumption 6. Also, in the case of Example 3, we have $G = d$ and $\beta = 2k$. Hence, the asymptotic simulation cost is at most
\[
\tilde{O} \left[ \frac{kd^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].
\]
We can see that choosing $k = 1$ gives the best upper bound. Finally, we note that if we substitute $\epsilon$ with $c/2$, all upper bounds of simulation cost under Assumption 6 also hold for the PCS-IZ guarantee.
4. Simulation Algorithms and Expected Simulation Costs for the General Case

In this section, we extend to the general $L^\natural$-convex function minimization problem with decision space $[N]^d$ for general large $N$ and $d$. We design simulation algorithms that achieve the PGS guarantee and prove upper bounds on the simulation costs.

As an extension to the methodology in Section 3, we first show that the Lovász extension in the neighborhood of each point can be pieced together to form a convex function on $\text{conv}(\mathcal{X}) = [1, N]^d$. We define the local neighborhood of each point $y \in [1, N-1]^d$ as the cube

$$C_y := y + [0,1]^d.$$ 

We denote the objective function $f(x)$ restricted to $C_y \cap \mathcal{X}$ as $f_y(x)$. For point $x \in C_y$, we denote $\alpha_x$ as a consistent permutation of $x - y$ in $\{0,1\}^d$, and for each $i \in \{0,1,\ldots,d\}$, the corresponding $i$-th neighboring point of $x$ is defined as

$$S^{x,i} := y + \sum_{j=1}^{i} e_{\alpha_x(j)}.$$ 

By the translation submodularity property of $L^\natural$-convex functions, we know function $f_y(x)$ is a submodular function on $y + \{0,1\}^d$ and its Lovász extension in $C_y$ can be calculated as

$$\tilde{f}_y(x) := f(S^{x,0}) + \sum_{i=1}^{d} \left[ f(S^{x,i}) - f(S^{x,i-1}) \right] x_{\alpha_x(i)}.$$ 

Now, we piece together the Lovász extension in each cube by defining

$$\tilde{f}(x) := \tilde{f}_y(x) \quad \forall x \in [1,N]^d, \ y \in [N-1]^d \quad \text{s.t.} \ x \in C_y.$$ 

The next theorem verifies the well-definedness and the convexity of $\tilde{f}$.

**Theorem 4.** The function $\tilde{f}(x)$ in (12) is well-defined and is convex on $\mathcal{X}$.

**Proof of Theorem 4.** The proof of Theorem 4 is given in EC.2.1.

Properties of the Lovász extension in Lemma 2 can be naturally extended to the convex extension $\tilde{f}(x)$. 

Lemma 5. Suppose Assumptions 1-5 hold. Then, the following properties of \( \tilde{f}(x) \) hold.

- For any \( x \in \mathcal{X} \), it holds \( \tilde{f}(x) = f(x) \).
- The minimizers of \( \tilde{f}_x \) satisfy \( \arg \min_{y \in [1,N]^d} \tilde{f}(y) = \arg \min_{y \in \mathcal{X}} f(y) \).
- For a point \( x \in C_y \), a subgradient \( g \in \partial \tilde{f}(x) \) is given by
  \[
g_{\alpha x(i)} := f(S^{x,i}) - f(S^{x,i-1}) \quad \forall i \in [d].
  \] (13)
- Subgradients of \( \tilde{f}_x \) satisfy
  \[\|g\|_1 \leq 3L/2 \quad \forall g \in \partial \tilde{f}(x), \; x \in \mathcal{X} .\]

Similar to the proof of Theorem 4, the subgradient given in (13) does not depend on the cube and the consistent permutation we choose. The subgradient estimators defined in (4) and (8) are still valid in the general case. Thus, changing the orthogonal projection to

\[\mathcal{P}(x) := (x \land N\mathbf{1}) \lor \mathbf{1} \quad \forall x \in \mathbb{R}^d,\]

Algorithm 2 can be directly extended to the general case and we get the counterpart to Theorem 2.

Theorem 5. Suppose Assumptions 1-5 hold and the subgradient estimator in (4) is used. If we choose

\[T = \tilde{\Theta}\left[\frac{dN^2}{\epsilon^2} \log \left(\frac{1}{\delta} \right)\right], \quad M = \tilde{\Theta}\left[\sqrt{\log \left(\frac{dN}{\epsilon} \right)}\right], \quad \eta = \frac{N}{M\sqrt{T}},\]

then Algorithm 2 returns an \((\epsilon, \delta)\)-PGS solution. Furthermore, we have

\[T(\epsilon, \delta, M\mathcal{C}) = O\left[\frac{d^2N^2}{\epsilon^2} \log \left(\frac{1}{\delta} \right) + \frac{d^3N^2}{\epsilon^2} \log \left(\frac{dN}{\epsilon} \right) + \frac{d^3N^2L^2}{\epsilon^2}\right] = \tilde{O}\left[\frac{d^2N^2}{\epsilon^2} \log \left(\frac{1}{\delta} \right)\right].\]

Proof of Theorem 5. The proof of Theorem 5 is given in EC.2.2.

Similarly, we can estimate the asymptotic simulation cost under Assumption 6.

Theorem 6. Suppose Assumptions 1-6 hold. If we skip the truncation step in Algorithm 2 (or equivalently set \( M = \infty \)) and choose

\[T = \tilde{\Theta}\left[\frac{(L+G)^2N^2}{\epsilon^2} \log \left(\frac{1}{\delta} \right)\right], \quad \eta = \sqrt{\frac{dN^2}{TG^2}},\]
then Algorithm 2 returns an \((\epsilon, \delta)\)-PGS solution. Furthermore, we have

\[
T(\epsilon, \delta, \mathcal{MC}) = O\left[\frac{\beta(L + G)^2N^2 + d}{\epsilon^2} \log\left(\frac{1}{\delta}\right) + \frac{G^2d^2N^2}{\epsilon^2} \log\left(\frac{1}{\delta}\right)\right].
\]

The above theorem can be proved in the same way as Theorem 3 and we omit the proof. We note that the step size \(\eta\) does not depend on \(N\) in this case.

For the PCS-IZ guarantee, we can choose \(\epsilon = c/2\) and Algorithm 2 will return a \((c, \delta)\)-PCS-IZ solution. Hence, the above asymptotic simulation costs also hold for the PCS-IZ guarantee.

However, with the priori knowledge about the indifference zone parameter, we can design an acceleration scheme similar to Xu et al. (2016) and reduce the dependence on \(N\) from \(N^2\) to \(\log(N)\). We first prove that the existence of indifference zone is equivalent to the so-called weak sharp minima condition of the convex extension. Also, we use the \(\ell_\infty\) norm in place of the \(\ell_2\) norm since the feasible set is a cube.

**Definition 5.** We say a function \(f(x) : \mathcal{X} \mapsto \mathbb{R}\) satisfies the **weak sharp minimum (WSM) condition**, if there exists a constant \(\eta > 0\) such that

\[
\|x - x^*\|_\infty \leq \eta (f(x) - f^*) \quad \forall x \in \mathcal{X},
\]

where \(x^*\) is the minimizer of \(f(x)\) and \(f^* := f(x^*)\).

The WSM condition is first defined in Burke and Ferris (1993), and is also called the polyhedral error bound condition in recent literature (Yang and Lin 2018). In addition, the WSM condition is a special case of the global growth condition in Xu et al. (2016) with \(\theta = 1\). The WSM condition can be used to leverage the distance between intermediate solutions and \((c, \delta)\)-PCS-IZ solutions.

The next theorem verifies that the WSM condition is equivalent to the existence of indifference zone.

**Theorem 7.** Suppose function \(f(x) : \mathcal{X} \mapsto \mathbb{R}\) is a \(L^n\)-convex function and \(\tilde{f}(x)\) is the convex extension on \([1, N]^d\). Given a constant \(c > 0\), function \(f(x) \in \mathcal{MC}_c\) if and only if \(\tilde{f}(x)\) satisfies the WSM condition with \(\eta = c^{-1}\).
Proof of Theorem 7. The proof of Theorem 7 is given in EC.2.3.

Using the WSM condition, we can accelerate Algorithm 2 by dynamically shrinking the searching space. To describe the shrinkage of searching space, we define the $\ell_\infty$-neighbourhood of point $x$ as

$$
N(x, a) := \{ y \in [1, N]^d : \| y - x \|_\infty \leq a \}
$$

and the orthogonal projection onto $N(x, a)$ as

$$
P_{x,a}(y) := (y \land (x + a)) \lor (x - a) \quad \forall x \in \mathbb{R}^d.
$$

Now we give the adaptive SSGD algorithm for the PCS-IZ guarantee.

\textbf{Algorithm 3} Adaptive SSGD method for PCS-IZ guarantee

\textbf{Input:} Model $\mathcal{X}, B_x, F(x, \xi_x)$, optimality guarantee parameter $\delta$, indifference zone parameter $c$.

\textbf{Output:} An $(c, \delta)$-PCS-IZ solution $x^*$ to problem (1).

1: Set the initial guarantee $\epsilon_0 \leftarrow cN/4$.
2: Set the number of epochs $E \leftarrow \lceil \log_2(N) \rceil + 1$.
3: Set the initial searching space $\mathcal{Y}_0 \leftarrow [1, N]^d$.
4: for $e = 0, \ldots, E - 1$ do
5: Use Algorithm 2 to get an $(\epsilon_e, \delta/(2E))$-PGS solution $x_e$ in $\mathcal{Y}_e$.
6: Update guarantee $\epsilon_{e+1} \leftarrow \epsilon_e/2$.
7: Update the searching space $\mathcal{Y}_{e+1} \leftarrow N(x_e, 2^{-e-2}N)$.
8: end for
9: Round $x_{E-1}$ to an integral point satisfying the $(c, \delta)$-PCS-IZ guarantee by Algorithm 4.

Basically, the algorithm finds a $(c/2, \delta)$-PGS solution and, with the assumption that the indifference zone parameter is $c$, the solution is satisfies the $(c, \delta)$-PCS-IZ guarantee. We prove that the expected simulation cost of Algorithm 3 has only $O(\log(N))$ dependence on $N$.

**Theorem 8.** Suppose Assumptions 4, 5 hold. Then, Algorithm 3 returns a $(c, \delta)$-PCS-IZ solution. Furthermore, we have

$$
T(\delta, MC_c) = O \left[ \frac{d^2 \log(N)}{c^2} \log \left( \frac{1}{\delta} \right) + \frac{d^3 \log(N)}{c^2} \log \left( \frac{d^2 N}{\epsilon^3} \right) + \frac{d^3 \log(N) L^2}{c^2} \right] = \tilde{O} \left[ \frac{d^2 \log(N)}{c^2} \log \left( \frac{1}{\delta} \right) \right].
$$
Proof of Theorem 8. The proof of Theorem 8 is given in EC.2.4.

Similarly, we can estimate the asymptotic simulation cost under Assumption 6 and we omit the proof.

Theorem 9. Suppose Assumptions 1-6 hold. Then, Algorithm 3 returns a \((c, \delta)-PCS-IZ\) solution. Furthermore, we have

\[
T(\delta, \mathcal{M}c_e) = \tilde{O}\left[ \frac{\beta(L+G)^2 \log(N) + d}{c^2} \log\left(\frac{1}{\delta}\right) \right].
\]

5. Lower Bound on Expected Simulation Cost

We derive lower bounds to the expected simulation cost for any simulation algorithm that can achieve the PGS guarantee. In this section, we prove that the expected simulation cost is lower bounded by \(O(de^{-2} \log(1/\delta))\). We acknowledge that the lower bound may not be exactly tight, but the proved lower bound results suggest the limits for all simulation algorithms to achieve PGS guarantee for general simulation optimization problems with convex structure.

To prove lower bounds, basically, we construct several convex models that have similar distributions but distinct optimal solutions. Hence, any simulation algorithms need a large number of simulation runs to differentiate these models. The difference between two models is characterized by the Kullback–Leibler (KL) divergence between their distributions. More rigorously, the information-theoretical inequality in Kaufmann et al. (2016) provides a systematic way to prove lower bounds of zeroth-order algorithms. Given a zeroth-order algorithm and a model \(M\), we denote \(N_x(\tau)\) as the number of times that \(F(x, \xi_x)\) is sampled when the algorithm terminates, where \(\tau\) is the stopping time of the algorithm. Then, it follows from the definition that

\[
\mathbb{E}_M[\tau] = \sum_{x \in \mathcal{X}} \mathbb{E}_M[N_x(\tau)],
\]

where \(\mathbb{E}_M\) is the expectation when the model \(M\) is given. Similarly, we can define \(\mathbb{P}_M\) as the probability when the model \(M\) is given. The following lemma is proved in Kaufmann et al. (2016) and is the major tool for deriving lower bounds in this paper.
Lemma 6. For any two models $M_1, M_2$ and any event $E \in \mathcal{F}_\tau$, we have

$$\sum_{x \in \mathcal{X}} \mathbb{E}_{M_1} [N_x(\tau)] \text{KL}(\nu_{1,x}, \nu_{2,x}) \geq d(\mathbb{P}_{M_1}(E), \mathbb{P}_{M_2}(E)), \quad (14)$$

where $d(x, y) := x \log(x/y) + (1 - x) \log((1 - x)/(1 - y))$, KL$(\cdot, \cdot)$ is the KL divergence and $\nu_{k,x}$ is the distribution of model $M_k$ at point $x$ for $k = 1, 2$.

We use the information-theoretical inequality $(14)$ as the major tool for deriving lower bounds and construct models that are hard to differentiate. We first reduce the construction of $L^2$-convex functions to the construction of submodular functions. Then, using the family of submodular functions defined in Graur et al. (2020), we can construct $d + 1$ submodular functions that have different optimal solutions and have the same value except on $d + 1$ potential solutions. Hence, the algorithm has to simulate enough samples on the $d + 1$ potential solutions to decide the optimal solution and the simulation cost is proportional to $d$.

Theorem 10. Suppose Assumptions 1-4 hold. We have

$$T(\epsilon, \delta, \mathcal{M}C) \geq \Theta \left[ \frac{d\sigma^2}{\epsilon^2} \log(\frac{1}{\delta}) \right].$$

**Proof of Theorem 10.** The proof of Theorem 10 is given in EC.3.1.

We note that the above lower bound is also true when Assumption 5 holds with $L \geq \epsilon/N$. In addition, the same construction as Theorem 10 leads to a lower bound on the expected simulation cost for the PCS-IZ guarantee as

$$T(\delta, \mathcal{M}C_c) \geq \Theta \left[ \frac{d\sigma^2}{c^2N^2} \log(\frac{1}{\delta}) \right].$$

6. Simulation Algorithms with Biased Gradient Information

In large-scale discrete simulation optimization, during a simulation run for performance evaluation at a given $d$-dimensional decision variable $x$, it is sometimes possible that the neighboring decision variables (those very close to $x$) can be evaluated simultaneously within the same simulation run for $x$ at marginal costs. See Jian (2017) and Jian et al. (2016) for a bike sharing discrete simulation...
optimization problem that adopts this feature. When the decision variable $x$ is in continuous space, this simultaneous simulation approach is called the *Infinitesimal Perturbation Analysis* (IPA) or the *Forward/Backward Automatic Differentiation*, in which a gradient estimator at $x$ can be obtained within the same simulation run for evaluation of $x$. In continuous decision space, such gradient estimators can be unbiased under Lipschitz continuity regularity conditions, though no general guarantees on bias exist when continuity fails. In contrast, for discrete simulation optimization problems, in particular for those where discrete decision variables do not easily relax to continuous variables, the gradient information becomes the difference of function value on $x$ and function value on the neighboring points of $x$. This gradient information is very difficult, if not impossible, to estimate without bias using only a single simulation run. In general, the system dynamics and logic are different for two different discrete decision variables even when they differ in only one coordinate. Therefore, in the simulation run for decision variable $x$, the simultaneous evaluation for neighbor decision variables may incur a bias. See Chapter 4 of Jian (2017) for a detailed discussion in the bike-sharing optimization as an example. Despite of the bias, the availability of such gradient information can potentially be beneficial when $d$ is large, because only one simulation run is needed to evaluate a biased version of a $d$-dimension gradient estimator. The gradient estimator can be usually obtained at a marginal cost that does not depend on the dimension $d$, which is much lower than the cost of constructing a finite difference gradient estimator.

In this section, we provide simulation algorithms to achieve PGS guarantee for discrete convex simulation optimization problems, when the gradient information is available (but possibly biased) within a simulation run at a cost that does not depend on dimension. We call this class of simulation algorithms which utilize the available gradient information *first-order algorithms*. We will show how the use of the gradient information reduces the expected simulation cost and how the bias existed in the gradient information affects the results. We first rigorously define the gradient information that can be obtained in simulation with discrete decision variables. Because of the discrete nature, the gradient information is technically noted as subgradient estimator. We start with the case
presuming no bias or correlation, as an illustration. We then extend to the realistic case with bias and correlation in the subgradient estimator.

**Assumption 7 (Subgradient estimator with no bias and correlation).** There exists a deterministic function $G(x, \eta_x): [1, N]^d \times Z \rightarrow \mathbb{R}^d$ such that

$$\langle \mathbb{E}[G(x, \eta_x)], x - x^* \rangle \geq \tilde{f}(x) - \tilde{f}(x^*) \quad \forall x \in [1, N]^d,$$

where $(Z, \mathcal{B}_Z)$ is a proper space that summarizes the randomness of $\eta_x$ in the sub-gradient estimator, $\tilde{f}(x)$ is the convex extension of $f(x)$ defined in (12) and $x^*$ is a minimizer of $f(x)$. Components of $G(x, \eta_x)$ are mutually independent and have sub-Gaussian distribution with parameter $\tilde{\sigma}^2$. Moreover, the simulation cost of obtaining $G(x, \eta_x)$ is at most $\gamma$ multiplying the simulation cost of evaluating $F(x, \xi_x)$.

If the gradient information that satisfies Assumption 7 is available, we can substitute the subgradient estimator (4) with $G(x, \eta_x)$ in Algorithms 2 and 3. The benefit is straightforward because there is no need to run $O(d)$ simulations to construct the subgradient estimator. The following result is the counterpart of Theorems 5 and 8.

**Theorem 11.** Suppose Assumptions 1-5, 7 hold and we use the subgradient estimator $G(x, \eta_x)$. If we choose $T, \eta, M$ as Theorem 5, then Algorithm 2 returns an $(\epsilon, \delta)$-PGS solution and we have

$$T(\epsilon, \delta, M) = \tilde{O} \left[ \frac{\beta dN^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].$$

Furthermore, if we choose $T, \eta, M$ as Theorem 8, then Algorithm 3 returns a $(c, \delta)$-PCS-IZ solution and we have

$$T(\delta, M) = \tilde{O} \left[ \frac{\beta d \log(N)}{c^2} \log \left( \frac{1}{\delta} \right) \right].$$

In the case when $\gamma = O(1)$, the simulation costs of Algorithms 2 and 3 are reduced by $O(d)$.

Next we consider cases when Assumption 7 does not hold and the gradient information that can be obtained within one simulation run is generally biased and has correlated components. The existence of correlation may increase the difficulty of analyzing the performance of simulation
algorithms. Moreover, the correlation will contribute to a larger overall variance of the norm of the subgradient estimator, which may adversely affect the simulation algorithm. On the bias side, if the bias in the subgradient estimator can be arbitrarily large, the sign of a subgradient estimator can even be flipped (see a counter example in Eckman and Henderson (2020)). In those cases, there is in general no guarantee for gradient-based algorithms even for convex problems. Examples in Ajalloeian and Stich (2020) also show that the biased gradient-based methods may not converge to the optimum or even dramatically diverge. To circumvent this challenge, some existing works on biased gradient-based methods require the objective function to be smooth and have additional benign geometrical properties, e.g., the strongly convexity or the Polyak-Łojasiewicz (PL) condition (Devolder et al. 2014, Chen and Luss 2018, Ajalloeian and Stich 2020, Hu et al. 2020). Since the convex extension of a general $L^b$-convex function is a piecewise linear function and is neither smooth nor strongly convex, these methods which require benign structure can not be applied to our case.

In the special case when the biased subgradient estimator of $f(x)$ is the unbiased subgradient estimator of a another function $h(x)$, we can view $h(x)$ as a perturbed version of $f(x)$. We define the Lovász extension of $h(x)$ in the same way and equivalently minimize the Lovász extension via the SSGD method. However, since function $h(x)$ may not be $L^b$-convex, the Lovász extension is a non-smooth and non-convex function and there is no guarantee on the complexity of the SSGD method (Davis et al. 2020, Daniilidis and Drusvyatskiy 2020). In Zhang et al. (2020), the authors proposed a stochastic normalized subgradient descent method with sample complexity $O(\epsilon^{-4})$ for finding a point with subgradient smaller than $\epsilon$. Under the assumption of weak convexity, algorithms with sample complexity of $O(\epsilon^{-2})$ have been proved in Davis and Drusvyatskiy (2018), Zhang and He (2018), Mai and Johansson (2020). On the other hand, to achieve the same sample complexity as convex optimization, it is proved that the perturbation $h(x) - f(x)$ should has order $O(1/d)$ (Belloni et al. 2015, Jin et al. 2018, Mangoubi and Vishnoi 2018). Finally, if function $h(x)$ has no spurious local minima, then we can apply the simulated annealing method with stochastic
oracles \cite{Bouttier2019}. The sample complexity is proved to be $O(\epsilon^{-3})$. However, the existence of the perturbed function $h(x)$ does not always hold and therefore we may not use the above methods.

The above discussion shows that some regularity assumptions on the bias are necessary for the applicability of gradient information to achieve PGS guarantee. Now, we describe a formal definition of biased subgradient estimator along with the assumption on bias. The key in the assumption is to regulate the relative magnitude of the bias, so that in expectation the bias does not flip the sign of the true subgradient at a decision variable. The use of common random variables whenever available in general can contribute to the validity of this assumption. As a comparison, \cite{Eckman2020} regulate the absolute value of the bias to provide guarantees for continuous stochastic optimization problems. To prepare notation, the set of neighboring decision variables of $x \in \mathcal{X}$ is defined as

$$
\mathcal{N}_x := \{x \pm e_S : S \subset [d] \} \cap \mathcal{X}.
$$

where $e_i$ is the $i$-th unit vector of $\mathbb{R}^d$ and $e_S$ is the indicator vector $\sum_{i \in S} e_i$. The following assumption describes the case that allows the gradient information to have bias and correlation among different directions.

**Assumption 8 (Subgradient estimator with bias and correlation.)** Given the bias ratio $a \in [0, 1)$, for any point $x \in \mathcal{X}$, there exists a deterministic function $H_x(y, \eta_y) : \mathcal{N}_x \times Z \mapsto \mathbb{R}$ such that

$$
|\mathbb{E}[H_x(y, \eta_y)] - [f(y) - f(x)]| \leq a \cdot |f(y) - f(x)|,
$$

(15)

where $\mathcal{N}_x$ is the set of neighboring points of $x$ and $(Z, \mathcal{B}_Z)$ is a proper space that summarizes the randomness of $G(x, \eta_x)$. Moreover, the marginal distribution for each $H_x(y, \eta_y)$ is sub-Gaussian with parameter $\tilde{\sigma}^2$ and the simulation cost of evaluating $H_x(y, \eta_y)$ for all $y \in \mathcal{N}_x$ is at most $\gamma$ multiplying the simulation cost of evaluating $F(x, \xi_x)$.\]
Under Assumption 8, the expectation of $\mathbb{E}[H_{x}(y, \eta_{y})]$ has the same sign as $f(y) - f(x)$ and, using Theorem 7.14 in Murota (2003), point $x \in \mathcal{X}$ is a minimizer of $f(x)$ if and only if

$$\mathbb{E}[H_{x}(y, \eta_{y})] \geq 0 \quad \forall y \in \mathcal{N}_{x}.$$ 

Furthermore, the following lemma shows that the lower bound of $\mathbb{E}[H_{x}(y, \eta_{y})]$ in $\mathcal{N}_{x}$ implies a global lower bound of $f(x)$.

**Lemma 7.** Suppose Assumptions 1-5 and 8 hold. If we have

$$\mathbb{E}[H_{x}(y, \eta_{y})] \geq -b \quad \forall y \in \mathcal{N}_{x}$$

for some constant $b \geq 0$, then it holds

$$f(y) \geq f(x) - \frac{2N}{1-a} \cdot b \quad \forall y \in \mathcal{X}.$$ 

**Proof of Lemma 7.** The proof of Theorem 7 is given in EC4.4. □

Hence, to find an $(\epsilon, \delta)$-PGS solution, it suffices to find point $x$ such that

$$\mathbb{E}[H_{x}(y, \eta_{y})] \geq -\frac{(1-a)\epsilon}{2N} \quad \forall y \in \mathcal{N}_{x}$$

holds with probability at least $1 - \delta$. Using the above observation, we give an algorithm for PGS guarantee using the biased subgradient estimator $H_{x}(y, \eta_{y})$. The algorithm can be seen as the stochastic version of the steepest descent method in Murota (2003) and we list the pseudo-code in Algorithm 4.

**Algorithm 4** Adaptive stochastic steepest descent method for PGS guarantee

**Input:** Model $\mathcal{X}, B_{x}, F(x, \xi_{x})$, optimality guarantee parameters $\epsilon, \delta$, biased subgradient estimator $H_{x}(y, \eta_{y})$, bias ratio $a$.

**Output:** An $(\epsilon, \delta)$-PGS solution $x^{*}$ to problem (1).

1. Choose the initial point $x^{0,0} \leftarrow (N/2, \ldots, N/2)^{T}$.
2. Set the initial confidence width threshold $h_{0} \leftarrow (1-a)L/12$.
3. Set maximal number of epochs $E \leftarrow \lceil \log_{2}(NL/\epsilon) \rceil$. 

4: Set maximal number of iterations $T \leftarrow (1 + a)/(1 - a) \cdot 6N$.

5: for $e = 0, 1, \ldots, E - 1$ do
6: for $t = 0, 1, \ldots, T - 1$ do
7: repeat simulate $H_{x,e,t}(y, \eta_y)$ for all $y \in N_{x,e,t}$
8: Compute the empirical mean $\hat{H}_{x,e,t}(y)$ using all simulated samples for all $y \in N_{x,e,t}$.
9: Compute the $1 - \delta/(ET)$ confidence interval
$$\left[ \hat{H}_{x,e,t}(y) - h_y, \hat{H}_{x,e,t}(y) + h_y \right] \forall y \in N_{x,e,t}.$$ 
10: until the confidence width $h_y \leq h_e$ for all $y \in N_{x,e,t}$
11: if $\hat{H}_{x,e,t}(y) \leq -2h_e$ for some $y \in N_{x,e,t}$ then
   $\triangleright$ This step takes $2^{d+1}$ arithmetic operations.
12: Update $x^{e,t+1} \leftarrow y$.
13: else if $\hat{H}_{x,e,t}(y) > -2h_e$ for some $y \in N_{x,e,t}$ then
14: break
15: end if
16: end for
17: Set $x^{e+1,0} \leftarrow x^{e,t}$ and $h_{e+1} \leftarrow h_e / 2$.
18: end for
19: Return $x^{E,0}$.

The following theorem verifies the correctness of Algorithm 4 and estimates its expected simulation cost.

**Theorem 12.** Suppose Assumptions 4, 5, 8 hold. Algorithm 4 returns an $(\epsilon, \delta)$-PGS solution and we have
$$T(\epsilon, \delta, MC) = O \left[ \frac{\gamma N^3}{(1 - a) \epsilon^2} \log \left( \frac{1}{\delta} \right) + \frac{\gamma N}{1 - a} \log \left( \frac{N}{\epsilon} \right) \right] = \tilde{O} \left[ \frac{\gamma N^3}{(1 - a)^3 \epsilon^2} \log \left( \frac{1}{\delta} \right) \right].$$

**Proof of Theorem 12.** The proof of Theorem 12 is given in EC.4.2. $\square$
We note that Algorithm 4 requires $2^{d+1}$ arithmetic operations for each iteration. Even though they share the same simulation logic, the memory cost may not be negligible, which may also incur additional computational cost of keeping track of large-scale vectors. There is then a trade-off between simulation costs and memory in general, which we do not exactly model in this work. To avoid exponentially many arithmetic operations and memory occupation in the steepest descent method, the comparison-based zeroth-order method in Agarwal et al. (2011) can be extended to our case and reduce the number of arithmetic operations to a polynomial in $d$. Also, we may consider using the following stochastic coordinate steepest descent method as a simple and fast implementation of Algorithms 4 and 5. Let $x^t$ be the current iteration point and we update by two steps.

1. Simulate $H_{x^t}(y, \eta_y)$ for all $y \in \{x^t \pm e_i, \ i \in [d]\}$ until the confidence interval is small enough.
2. If for some $y \in \{x^t \pm e_i, \ i \in [d]\}$, we know $f(y) < f(x^t)$ holds with high probability, then update $x^{t+1} = y$; otherwise if $f(y) \geq f(x^t) - O(\epsilon)$ holds for all $y \in \{x^t \pm e_i, \ i \in [d]\}$ with high probability, then we terminate the iteration and return $x^t$ as the solution.

We can see that the number of arithmetic operations for each iteration is $O(d)$. Also, an analogous method utilizing $O(d)$ neighboring points in constructing gradient is shown to have good empirical performance in Jian (2017). However, theoretically, without extra assumptions on the problem structure, the stopping guarantee $f(y) \geq f(x) - O(\epsilon)$ for all $y \in \{x^t \pm e_i, \ i \in [d]\}$ can not ensure the approximate optimality of solution $x$. We give a counterexample to show that $f(y) \geq f(x)$ for all $y \in \{x^t \pm e_i, \ i \in [d]\}$ can not ensure the optimality of solution $x$.

**Example 4.** We consider the case when $d = 2$ and $N = 3$. Define the objective function as

$$f(x, y) := 2|x - y| - |x + y - 2| \quad \forall (x, y) \in \{1, 2, 3\}^2.$$  

We can verify that $f(x, y)$ is a $L^\natural$-convex function and its minimizer is $(3, 3)$ with optimal value $-4$. Considering point $(2, 2)$, we can calculate that

$$f(2, 2) = -2, \ f(1, 2) = 1, \ f(3, 2) = -1, \ f(2, 1) = 1, \ f(2, 3) = -1.$$ 

Hence, the guarantee is satisfied at $(2, 2)$ but the point is not a minimizer of $f(x)$.  


We leave as future work for the study of general theoretical guarantees for simulation algorithms that use more flexible biased gradient estimators.

Intuitively, in the case when the indifference zone parameter $c$ is known, we can prove that choosing $\epsilon = Nc$ is enough for the $(c, \delta)$-PCS-IZ guarantee. We give the stochastic steepest descent method for the PCS-IZ guarantee in Algorithm 5.

Algorithm 5 Adaptive stochastic steepest descent method for PCS-IZ guarantee

**Input:** Model $\mathcal{X}, B_x, F(x, \xi_x)$, optimality guarantee parameter $\delta$, indifference zone parameter $c$, biased subgradient estimator $H_x(y, \eta_y)$, bias ratio $a$.

**Output:** A $(c, \delta)$-PCS-IZ solution $x^*$ to problem (1).

1: Set the initial confidence width threshold $h \leftarrow (1 - a)c/12$.
2: Set maximal number of iterations $T \leftarrow (1 + a)/(1 - a) \cdot 12N$.
3: Use Algorithm 4 to find an $(Nc, \delta/2)$-PGS solution.
4: for $t = 0, 1, \ldots, T - 1$ do
5: repeat simulate $H_x(y, \eta_y)$ for all $y \in \mathcal{N}_{x^t}$
6: Compute the empirical mean $\hat{H}_x(y)$ using all simulated samples for all $y \in \mathcal{N}_{x^t}$.
7: Compute the $1 - \delta/(2T)$ confidence interval
   
   $\left[\hat{H}_x(y) - h_y, \hat{H}_x(y) + h_y\right] \quad \forall y \in \mathcal{N}_{x^t}$.

8: until the confidence width $h_y \leq h$ for all $y \in \mathcal{N}_{x^t}$
9: if $\hat{H}_x(y) \leq -2h$ for some $y \in \mathcal{N}_{x^t}$ then \hspace{1em} $\triangleright$ This step takes $2^{d+1}$ arithmetic operations.
10: Update $x^{t+1} \leftarrow y$.
11: else if $\hat{H}_x(y) > -2h$ for some $y \in \mathcal{N}_{x^t}$ then
12: break
13: end if
14: end for
15: Return $x^t$. 
The following theorem verifies the correctness of Algorithm 5 and estimates its asymptotic simulation cost.

**Theorem 13.** Suppose Assumptions 1-5, 8 hold. Algorithm 5 returns an $(c,\delta)$-PCS-IZ solution and we have

\[
T(\delta, MC_c) = O\left[ \frac{\gamma N}{(1-a)^3 c^2} \log\left(\frac{1}{\delta}\right) + \frac{\gamma N}{1-a} \max\left\{ \log\left(\frac{1}{c}\right), 1 \right\} \right] = \tilde{O}\left[ \frac{\gamma N}{(1-a)^3 c^2} \log\left(\frac{1}{\delta}\right) \right].
\]

**Proof of Theorem 13.** The proof of Theorem 13 is given in EC.4.3.

7. Conclusion

We propose computationally efficient simulation algorithms for large-scale simulation optimization problems that have high-dimensional discrete decision space in presence of a convex structure. For a user-specified precision level, the proposed simulation algorithms are guaranteed to find a solution that is close to the optimal within the precision level with desired high probability. We provide upper bounds on simulation costs for the proposed simulation algorithms. In this work, we mainly focus on algorithm design and theoretical guarantees. In future work, we plan to test the empirical performance of the proposed simulation algorithms on large-scale convex problems. Also, we seek to design better simulation algorithms that provide simulation costs with matching upper and lower bounds.

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**References**

Agarwal A, Foster DP, Hsu DJ, Kakade SM, Rakhlin A (2011) Stochastic convex optimization with bandit feedback. Advances in Neural Information Processing Systems, 1035–1043.

Agrawal S, Juneja S, Glynn P (2020) Optimal $\delta$-correct best-arm selection for heavy-tailed distributions. Algorithmic Learning Theory, 61–110.

Ajalleian A, Stich SU (2020) Analysis of sgd with biased gradient estimators. arXiv preprint arXiv:2008.00051.
Altman E, Gaujal B, Hordijk A (2003) Discrete-event control of stochastic networks: Multimodularity and regularity (springer).

Audibert JY, Bubeck S (2010) Best arm identification in multi-armed bandits.

Axelrod B, Liu YP, Sidford A (2020) Near-optimal approximate discrete and continuous submodular function minimization. Proceedings of the Fourteenth Annual ACM-SIAM Symposium on Discrete Algorithms, 837–853 (SIAM).

Bach F (2019) Submodular functions: from discrete to continuous domains. Mathematical Programming 175(1-2):419–459.

Balasubramanian K, Ghadimi S (2018) Zeroth-order nonconvex stochastic optimization: Handling constraints, high-dimensionality and saddle-points. arXiv preprint arXiv:1809.06474.

Bechhofer RE (1954) A single-sample multiple decision procedure for ranking means of normal populations with known variances. The Annals of Mathematical Statistics 16–39.

Belloni A, Liang T, Narayanan H, Rakhlin A (2015) Escaping the local minima via simulated annealing: Optimization of approximately convex functions. Conference on Learning Theory, 240–265.

Borjesson P, Sundberg CE (1979) Simple approximations of the error function q (x) for communications applications. IEEE Transactions on Communications 27(3):639–643.

Bouttier C, Gavra I (2019) Convergence rate of a simulated annealing algorithm with noisy observations. The Journal of Machine Learning Research 20(1):127–171.

Bubeck S, Munos R, Stoltz G (2011) Pure exploration in finitely-armed and continuous-armed bandits. Theoretical Computer Science 412(19):1832–1852.

Burke JV, Ferris MC (1993) Weak sharp minima in mathematical programming. SIAM Journal on Control and Optimization 31(5):1340–1359.

Carpentier A, Locatelli A (2016) Tight (lower) bounds for the fixed budget best arm identification bandit problem. Conference on Learning Theory, 590–604.

Chen CH (1996) A lower bound for the correct subset-selection probability and its application to discrete-event system simulations. IEEE transactions on automatic control 41(8):1227–1231.
Chen Ch, Lee LH (2011) Stochastic simulation optimization: an optimal computing budget allocation, volume 1 (World scientific).

Chen CH, Lin J, Yücesan E, Chick SE (2000) Simulation budget allocation for further enhancing the efficiency of ordinal optimization. *Discrete Event Dynamic Systems* 10(3):251–270.

Chen J, Luss R (2018) Stochastic gradient descent with biased but consistent gradient estimators. *arXiv preprint arXiv:1807.11880*.

Chen L, Li J, Qiao M (2017) Towards instance optimal bounds for best arm identification. *Conference on Learning Theory*, 535–592.

Chen X, Ankenman BE, Nelson BL (2013) Enhancing stochastic kriging metamodels with gradient estimators. *Operations Research* 61(2):512–528.

Chen X, Zhou E, Hu J (2018) Discrete optimization via gradient-based adaptive stochastic search methods. *IISE Transactions* 50(9):789–805.

Chick SE (2006) Subjective probability and bayesian methodology. *Handbooks in Operations Research and Management Science* 13:225–257.

Chick SE, Inoue K (2001) New two-stage and sequential procedures for selecting the best simulated system. *Operations Research* 49(5):732–743.

Daniilidis A, Drusvyatskiy D (2020) Pathological subgradient dynamics. *SIAM Journal on Optimization* 30(2):1327–1338.

Davis D, Drusvyatskiy D (2018) Stochastic subgradient method converges at the rate $o(k^{-1/4})$ on weakly convex functions. *arXiv preprint arXiv:1802.02988*.

Davis D, Drusvyatskiy D, Kakade S, Lee JD (2020) Stochastic subgradient method converges on tame functions. *Foundations of computational mathematics* 20(1):119–154.

Degene R, Koolen WM (2019) Pure exploration with multiple correct answers. *Advances in Neural Information Processing Systems*, 14591–14600.

Degene R, Koolen WM, Ménard P (2019) Non-asymptotic pure exploration by solving games. *Advances in Neural Information Processing Systems*, 14492–14501.
Devolder O, Glineur F, Nesterov Y (2014) First-order methods of smooth convex optimization with inexact oracle. *Mathematical Programming* 146(1-2):37–75.

Duchi JC, Jordan MI, Wainwright MJ, Wibisono A (2015) Optimal rates for zero-order convex optimization: The power of two function evaluations. *IEEE Transactions on Information Theory* 61(5):2788–2806.

Eckman DJ, Henderson SG (2018a) Fixed-confidence, fixed-tolerance guarantees for selection-of-the-best procedures. Technical report, Working paper, Cornell University, School of Operations Research and . . .

Eckman DJ, Henderson SG (2018b) Guarantees on the probability of good selection. *2018 Winter Simulation Conference (WSC)*, 351–365 (IEEE).

Eckman DJ, Henderson SG (2020) Biased gradient estimators in simulation optimization. Bae KH, Feng B, Kim S, Lazarova-Molnar S, Zheng Z, Roeder T, Thiesing R, eds., *Proceedings of the 2020 Winter Simulation Conference*, Submitted (Piscataway NJ: IEEE).

Eckman DJ, Plumlee M, Nelson BL (2020) Plausible screening using functional properties for simulations with large solution spaces, working paper.

Even-Dar E, Mannor S, Mansour Y (2002) Pac bounds for multi-armed bandit and markov decision processes. *International Conference on Computational Learning Theory*, 255–270 (Springer).

Even-Dar E, Mannor S, Mansour Y (2006) Action elimination and stopping conditions for the multi-armed bandit and reinforcement learning problems. *Journal of machine learning research* 7(Jun):1079–1105.

Fan W, Hong LJ, Nelson BL (2016) Indifference-zone-free selection of the best. *Operations Research* 64(6):1499–1514.

Favati P (1990) Convexity in nonlinear integer programming. *Ricerca operativa* 53:3–44.

Frazier P, Powell W, Dayanik S (2009) The knowledge-gradient policy for correlated normal beliefs. *INFORMS journal on Computing* 21(4):599–613.

Frazier PI (2014) A fully sequential elimination procedure for indifference-zone ranking and selection with tight bounds on probability of correct selection. *Operations Research* 62(4):926–942.

Freund D, Henderson SG, Shmoys DB (2017) Minimizing multimodular functions and allocating capacity in bike-sharing systems. *International Conference on Integer Programming and Combinatorial Optimization*, 186–198 (Springer).
Fu MC (2002) Optimization for simulation: Theory vs. practice. *INFORMS Journal on Computing* 14(3):192–215.

Fu MC, Qu H (2014) Regression models augmented with direct stochastic gradient estimators. *INFORMS Journal on Computing* 26(3):484–499.

Fujishige S (1984) Theory of submodular programs: A fenchel-type min-max theorem and subgradients of submodular functions. *Mathematical Programming* 29(2):142–155.

Fujishige S (2005) *Submodular functions and optimization* (Elsevier).

Futschik A, Pflug G (1995) Confidence sets for discrete stochastic optimization. *Annals of Operations Research* 56(1):95–108.

Futschik A, Pflug GC (1997) Optimal allocation of simulation experiments in discrete stochastic optimization and approximative algorithms. *European Journal of Operational Research* 101(2):245–260.

Gao S, Chen W, Shi L (2017) A new budget allocation framework for the expected opportunity cost. *Operations Research* 65(3):787–803.

Garivier A, Kaufmann E (2016) Optimal best arm identification with fixed confidence. *Conference on Learning Theory*. 998–1027.

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

Graur A, Pollner T, Ramaswamy V, Weinberg SM (2020) New query lower bounds for submodular function minimization. *11th Innovations in Theoretical Computer Science Conference (ITCS 2020)* (Schloss Dagstuhl-Leibniz-Zentrum für Informatik).

Gutjahr WJ, Pflug GC (1996) Simulated annealing for noisy cost functions. *Journal of global optimization* 8(1):1–13.

Hazan E, Kale S (2011) Beyond the regret minimization barrier: an optimal algorithm for stochastic strongly-convex optimization. *Proceedings of the 24th Annual Conference on Learning Theory*. 421–436.

Homem-de Mello T, Bayraksan G (2014) Monte carlo sampling-based methods for stochastic optimization. *Surveys in Operations Research and Management Science* 19(1):56–85.
Hong LJ, Fan W, Luo J (2020) Review on ranking and selection: A new perspective. arXiv preprint arXiv:2008.00249.

Hong LJ, Nelson BL (2006) Discrete optimization via simulation using compass. Operations Research 54(1):115–129.

Hong LJ, Nelson BL, Xu J (2010) Speeding up compass for high-dimensional discrete optimization via simulation. Operations Research Letters 38(6):550–555.

Hong LJ, Nelson BL, Xu J (2015) Discrete optimization via simulation. Handbook of simulation optimization, 9–44 (Springer).

Hu J, Fu MC, Marcus SI (2007) A model reference adaptive search method for global optimization. Operations Research 55(3):549–568.

Hu J, Fu MC, Marcus SI, et al. (2008) A model reference adaptive search method for stochastic global optimization. Communications in Information & Systems 8(3):245–276.

Hu Y, Zhang S, Chen X, He N (2020) Biased stochastic gradient descent for conditional stochastic optimization. arXiv preprint arXiv:2002.10790.

Hunter SR, Nelson BL (2017) Parallel ranking and selection. Advances in Modeling and Simulation, 249–275 (Springer).

Ito S (2019) Submodular function minimization with noisy evaluation oracle. Advances in Neural Information Processing Systems, 12103–12113.

Jamieson K, Malloy M, Nowak R, Bubeck S (2014) lil’ucb: An optimal exploration algorithm for multi-armed bandits. Conference on Learning Theory, 423–439.

Jian N (2017) Exploring and exploiting structure in large scale simulation optimization. Ph. D. thesis Operations Research and Information Engineering, Cornell University, Ithaca NY.

Jian N, Freund D, Wiberg HM, Henderson SG (2016) Simulation optimization for a large-scale bike-sharing system. 2016 Winter Simulation Conference (WSC), 602–613 (IEEE).

Jin C, Liu LT, Ge R, Jordan MI (2018) On the local minima of the empirical risk. Advances in neural information processing systems, 4896–4905.
Kalyanakrishnan S, Stone P (2010) Efficient selection of multiple bandit arms: theory and practice. Proceedings of the 27th International Conference on International Conference on Machine Learning, 511–518.

Kalyanakrishnan S, Tewari A, Auer P, Stone P (2012) Pac subset selection in stochastic multi-armed bandits. ICML, volume 12, 655–662.

Karnin Z, Koren T, Somekh O (2013) Almost optimal exploration in multi-armed bandits. International Conference on Machine Learning, 1238–1246.

Kaufmann E, Cappé O, Garivier A (2014) On the complexity of a/b testing. Conference on Learning Theory, 461–481.

Kaufmann E, Cappé O, Garivier A (2016) On the complexity of best-arm identification in multi-armed bandit models. The Journal of Machine Learning Research 17(1):1–42.

Kaufmann E, Kalyanakrishnan S (2013) Information complexity in bandit subset selection. Conference on Learning Theory, 228–251.

Kim SH (2005) Comparison with a standard via fully sequential procedures. ACM Transactions on Modeling and Computer Simulation (TOMACS) 15(2):155–174.

Kim SH, Nelson BL (2001) A fully sequential procedure for indifference-zone selection in simulation. ACM Transactions on Modeling and Computer Simulation (TOMACS) 11(3):251–273.

Kim SH, Nelson BL (2006) Selecting the best system. Handbooks in operations research and management science 13:501–534.

Kleywegt AJ, Shapiro A, Homem-de Mello T (2002) The sample average approximation method for stochastic discrete optimization. SIAM Journal on Optimization 12(2):479–502.

Larson J, Menickelly M, Wild SM (2019) Derivative-free optimization methods. arXiv preprint arXiv:1904.11585.

Lattimore T, Szepesvári C (2020) Bandit algorithms (Cambridge University Press).

L’Ecuyer P (1990) A unified view of the ipa, sf, and lr gradient estimation techniques. Management Science 36(11):1364–1383.
Lee YT, Sidford A, Wong SCw (2015) A faster cutting plane method and its implications for combinatorial and convex optimization. *2015 IEEE 56th Annual Symposium on Foundations of Computer Science*, 1049–1065 (IEEE).

Lim E (2012) Stochastic approximation over multidimensional discrete sets with applications to inventory systems and admission control of queueing networks. *ACM Transactions on Modeling and Computer Simulation (TOMACS)* 22(4):1–23.

Lovász L (1983) Submodular functions and convexity. *Mathematical programming the state of the art*, 235–257 (Springer).

Luo J, Hong LJ, Nelson BL, Wu Y (2015) Fully sequential procedures for large-scale ranking-and-selection problems in parallel computing environments. *Operations Research* 63(5):1177–1194.

Ma S, Henderson SG (2017) An efficient fully sequential selection procedure guaranteeing probably approximately correct selection. *2017 Winter Simulation Conference (WSC)*, 2225–2236 (IEEE).

Ma S, Henderson SG (2019) Predicting the simulation budget in ranking and selection procedures. *ACM Transactions on Modeling and Computer Simulation* 29(3):Article 14, 1–25.

Mai VV, Johansson M (2020) Convergence of a stochastic gradient method with momentum for nonsmooth nonconvex optimization. *arXiv preprint arXiv:2002.05466*.

Mangoubi O, Vishnoi NK (2018) Convex optimization with unbounded nonconvex oracles using simulated annealing. *Conference On Learning Theory*, 1086–1124 (PMLR).

Mannor S, Tsitsiklis JN (2004) The sample complexity of exploration in the multi-armed bandit problem. *Journal of Machine Learning Research* 5(Jun):623–648.

Murota K (2003) Discrete convex analysis. *Society for Industrial and Applied Mathematics* (Citeseer).

Nelson BL (2010) Optimization via simulation over discrete decision variables. *Risk and Optimization in an Uncertain World*, 193–207 (Informs).

Nemirovsky AS, Yudin DB (1983) Problem complexity and method efficiency in optimization.

Nesterov Y (2018) *Lectures on convex optimization*, volume 137 (Springer).

Nesterov Y, Spokoiny V (2017) Random gradient-free minimization of convex functions. *Foundations of Computational Mathematics* 17(2):527–566.
Ni EC, Ciocan DF, Henderson SG, Hunter SR (2017) Efficient ranking and selection in high performance computing environments. Operations Research 65(3):821–836.

Park C, Kim SH (2015) Penalty function with memory for discrete optimization via simulation with stochastic constraints. Operations Research 63(5):1195–1212.

Park C, Telci IT, Kim SH, Aral MM (2014) Designing an optimal water quality monitoring network for river systems using constrained discrete optimization via simulation. Engineering Optimization 46(1):107–129.

Peng Y, Chong EK, Chen CH, Fu MC (2018) Ranking and selection as stochastic control. IEEE Transactions on Automatic Control 63(8):2359–2373.

Qin C, Klabjan D, Russo D (2017) Improving the expected improvement algorithm. Advances in Neural Information Processing Systems, 5381–5391.

Qu H, Fu MC (2014) Gradient extrapolated stochastic kriging. ACM Transactions on Modeling and Computer Simulation (TOMACS) 24(4):1–25.

Russo D (2020) Simple bayesian algorithms for best-arm identification. Operations Research.

Salemi PL, Song E, Nelson BL, Staum J (2019) Gaussian markov random fields for discrete optimization via simulation: Framework and algorithms. Operations Research 67(1):250–266.

Semelhago M, Nelson BL, Song E, Wächter A (2020) Rapid discrete optimization via simulation with gaussian markov random fields. INFORMS journal on Computing Articles in Advance.

Sen S, Higle JL (2001) Stabilization of cutting plane algorithms for stochastic linear programming problems. Stabilization of Cutting Plane Algorithms for Stochastic Linear Programming Problems, 2434–2440 (Boston, MA: Springer US), ISBN 978-0-306-48332-5, URL http://dx.doi.org/10.1007/0-306-48332-7_482

Shaked M, Shanthikumar JG (1988) Stochastic convexity and its applications. Advances in Applied Probability 20(2):427–446.

Shamir O (2011) A variant of azuma’s inequality for martingales with subgaussian tails. arXiv preprint arXiv:1110.2392.
Singhvi D, Singhvi S, Frazier PI, Henderson SG, O’Mahony E, Shmoys DB, Woodard DB (2015) Predicting bike usage for new york city’s bike sharing system. *AAAI Workshop: Computational Sustainability* (Citeseer).

Sun L, Hong LJ, Hu Z (2014) Balancing exploitation and exploration in discrete optimization via simulation through a gaussian process-based search. *Operations Research* 62(6):1416–1438.

Wang H, Pasupathy R, Schmeiser BW (2013) Integer-ordered simulation optimization using r-spline: Retrospective search with piecewise-linear interpolation and neighborhood enumeration. *ACM Transactions on Modeling and Computer Simulation (TOMACS)* 23(3):1–24.

Wang T, Xu J, Hu JQ, Chen CH (2020) Optimal computing budget allocation for regression with gradient information. to appear.

Wolff RW, Wang CL (2002) On the convexity of loss probabilities. *Journal of applied probability* 402–406.

Wu D, Zhou E (2018) Analyzing and provably improving fixed budget ranking and selection algorithms. *arXiv preprint arXiv:1811.12183*.

Xu J, Nelson BL, Hong JL (2010) Industrial strength compass: A comprehensive algorithm and software for optimization via simulation. *ACM Transactions on Modeling and Computer Simulation (TOMACS)* 20(1):1–29.

Xu Y, Lin Q, Yang T (2016) Accelerated stochastic subgradient methods under local error bound condition. *arXiv preprint arXiv:1607.01027*.

Yang T, Lin Q (2018) Rsg: Beating subgradient method without smoothness and strong convexity. *The Journal of Machine Learning Research* 19(1):236–268.

Yu X, Shao H, Lyu MR, King I (2018) Pure exploration of multi-armed bandits with heavy-tailed payoffs. *UAI*, 937–946.

Zhang J, Lin H, Sra S, Jadbabaie A (2020) On complexity of finding stationary points of nonsmooth non-convex functions. *arXiv preprint arXiv:2002.04130*.

Zhang S, He N (2018) On the convergence rate of stochastic mirror descent for nonsmooth nonconvex optimization. *arXiv preprint arXiv:1806.04781*. 
Zinkevich M (2003) Online convex programming and generalized infinitesimal gradient ascent. *Proceedings of the 20th international conference on machine learning (icml-03)*, 928–936.
Supplementary Material – Proofs of Statements

EC.1. Proofs in Section 3

EC.1.1. Proof of Theorem 1

Proof of Theorem 1. We denote the optimal value of $f(x)$ as $f^*$. Since point $\bar{x}$ satisfies the $(\epsilon/2, \delta/2)$-PGS guarantee, we have

$$\tilde{f}(\bar{x}) - f^* \leq \epsilon/2$$

holds with probability at least $1 - \delta/2$. We assume this event happens in the following of this proof.

Let $S^0, S^1, \ldots, S^d$ be the neighboring points of $\bar{x}$. Using the expression of the Lovász extension in (6), we know there exists an $\epsilon$-optimal solution among $S^0, S^1, \ldots, S^d$. We denote the $\epsilon$-optimal solution and the solution returned by Algorithm 1 as $S^*$ and $x^*$, respectively. By the definition of confidence intervals, it holds

$$|\hat{F}_n(S^*) - f(S^*)| \leq \epsilon/4, \quad |\hat{F}_n(x^*) - f(x^*)| \leq \epsilon/4$$

with probability at least $1 - \delta/2$. Under this event, we know

$$f(x^*) - f^* \leq \hat{F}_n(x^*) - f^* + \epsilon/4 \leq \hat{F}_n(S^*) - f^* + \epsilon/4 \leq f(S^*) - f^* + \epsilon/2 \leq \epsilon,$$

which implies that $x^* \in X$ is an $\epsilon$-optimal solution and the probability is at least $1 - \delta/2 - \delta/2 = 1 - \delta$. Hence, we know $x^*$ is an $(\epsilon, \delta)$-PGS solution to problem (1).

Now, we estimate the simulation cost of Algorithm 1. By Hoeffding bound, simulating

$$\frac{32}{\epsilon^2} \log \left( \frac{8}{\delta} \right)$$

times on each neighboring point is enough to achieve $1 - \delta/4$ confidence width $\epsilon/4$. Hence, the simulation cost of Algorithm 1 is at most

$$\frac{32(d + 1)}{\epsilon^2} \log \left( \frac{8}{\delta} \right) = O \left[ \frac{d}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].$$

$\square$
EC.1.2. Proof of Theorem 2

Since the stochastic subgradient \( \hat{g}^t \) is truncated, the stochastic subgradient used for updating, namely \( \tilde{g}^t \), is not unbiased. We define the bias at each step as

\[
b_t := \mathbb{E} \left[ \tilde{g}^t \mid x^0, x^1, \ldots, x^t \right] - g^t \quad \forall t \in \{0, 1, \ldots, T - 1\}.
\]

First, we bound the \( \ell_1 \)-norm of the bias.

**Lemma EC.1.** Suppose Assumptions 1-5 hold. If we have

\[
M \geq 2\sigma \cdot \sqrt{\log \left( \frac{4\sigma d T}{\epsilon} \right)} = \Theta \left( \sqrt{\log \left( \frac{dT}{\epsilon} \right)} \right), \quad T \geq \frac{2\epsilon}{\sigma},
\]

then it holds

\[
\|b^t\|_1 \leq \frac{\epsilon}{2T} \quad \forall t \in \{0, 1, \ldots, T - 1\}.
\]

**Proof.** Let \( \alpha_t \) be a consistent permutation of \( x^t \) and \( S^{t,i} \) be the corresponding \( i \)-th neighboring points. We only need to prove

\[
|b^t_{\alpha_t(i)}| \leq \frac{\epsilon}{2dT} \quad \forall i \in [d].
\]

We define two random variables

\[
Y_1 := F \left( S^{t,i}, \xi^1_i \right) - f \left( S^{t,i} \right), \quad Y_2 := F \left( S^{t,i-1}, \xi^2_{i-1} \right) - f \left( S^{t,i-1} \right).
\]

By Assumption 3 both \( Y_1 \) and \( Y_2 \) are independent and sub-Gaussian with parameter \( \sigma^2 \). Hence, we know

\[
b^t_{\alpha_t(i)} = \mathbb{E} \left[ \hat{g}^t_{\alpha_t(i)} - g^t_{\alpha_t(i)} \right] = \mathbb{E} \left[ (Y_1 + Y_2) \cdot 1_{-M \leq Y_1 + Y_2 \leq M} \right] + \mathbb{E} \left[ M \cdot 1_{Y_1 + Y_2 > M} \right] + \mathbb{E} \left[ -M \cdot 1_{Y_1 + Y_2 < -M} \right]
\]

\[
= \mathbb{E} \left[ (M - Y_1 - Y_2) \cdot 1_{Y_1 + Y_2 > M} \right] + \mathbb{E} \left[ -(M + Y_1 + Y_2) \cdot 1_{Y_1 + Y_2 < -M} \right],
\]

where the second step is from \( \mathbb{E}[Y_1] = \mathbb{E}[Y_2] = 0 \). Taking the absolute value on both sides, we get

\[
|b^t_{\alpha_t(i)}| \leq \mathbb{E} \left[ (Y_1 + Y_2 - M) \cdot 1_{Y_1 + Y_2 > M} \right] + \mathbb{E} \left[ -(M + Y_1 + Y_2) \cdot 1_{Y_1 + Y_2 < -M} \right] \quad \text{(EC.1)}
\]

\[
= \mathbb{E} \left[ (Y - M) \cdot 1_{Y > M} \right] + \mathbb{E} \left[-(Y + M) \cdot 1_{Y < -M} \right].
\]
where we define the random variable $Y := Y_1 + Y_2$. Since $Y_1, Y_2$ are independent, random variable $Y$ is sub-Gaussian with parameter $2\sigma^2$. Let $F(y) := \mathbb{P}[Y \leq y]$ be the distribution function of $Y$.

Then, we have

$$\mathbb{E}[(Y - M) \cdot 1_{Y > M}] = \int_M^\infty (y - M) \, dF(y) = \int_M^\infty (1 - F(y)) \, dy. \quad \text{(EC.2)}$$

By the Hoeffding bound, we know

$$1 - F(y) = \mathbb{P}[Y > y] \leq \exp\left(-\frac{y^2}{4\sigma^2}\right) \quad \forall y \geq 0.$$ 

Using the upper bound for $Q$-function in [Borjesson and Sundberg (1979)], it holds that

$$\int_M^\infty 1 - F(y) \, dy \leq \int_M^\infty \exp\left(-\frac{y^2}{4\sigma^2}\right) \, dy \leq \frac{2\sigma^2}{M} \exp\left(-\frac{M^2}{4\sigma^2}\right).$$

By the choice of $M$, we know

$$M \geq 2\sigma \sqrt{\log(8d)} \geq 2\sigma \quad \text{and} \quad \sigma \exp(-M^2/4\sigma^2) \leq \frac{\epsilon}{4dT},$$

which implies that

$$\int_M^\infty 1 - F(y) \, dy \leq \frac{2\sigma^2}{M} \exp(-M^2/4\sigma^2) \leq \frac{\epsilon}{4dT}.$$

Substituting the above inequality into (EC.2), we have

$$\mathbb{E}[(Y - M) \cdot 1_{Y > M}] \leq \frac{\epsilon}{4dT}.$$ 

Considering $-Y$ in the same way, we can prove

$$\mathbb{E}[-(Y + M) \cdot 1_{Y < -M}] \leq \frac{\epsilon}{4dT}.$$ 

Substituting the last two estimates into inequality (EC.1), we know

$$|b^t_{\alpha_t(i)}| \leq \frac{\epsilon}{2dT}.$$ 

Next, we show that $(g^t + b^t - \tilde{g}^t, x^t - x^*)$ forms a martingale sequence and use Azuma’s inequality to bound the deviation, where $x^*$ is a minimizer of $f(x)$. 

Lemma EC.2. Suppose Assumptions 4,5 hold and let \( x^* \) be a minimizer of \( f(x) \). The sequence

\[ X_t := \langle g^t + b^t - \tilde{g}^t, x^t - x^* \rangle \quad t = 0, 1, \ldots, T - 1 \]

forms a martingale difference sequence. Furthermore, if we have

\[ M = \max \left\{ L, 2\sigma \cdot \sqrt{\log \left( \frac{4\sigma dT}{\epsilon} \right)} \right\} = \tilde{\Theta} \left[ \frac{\sqrt{\log(dT)}}{\sigma} \right], \quad T \geq 2\epsilon / \sigma, \]

then it holds

\[ \frac{1}{T} \sum_{t=0}^{T-1} X_t \leq \sqrt{\frac{224d\sigma^2}{T \log(1/\delta)}} \]

with probability at least \( 1 - \delta \).

Proof. Let \( F_t \) be the filtration generated by \( x_0, x_1, \ldots, x_t \). By the definition of \( b^t \), we know

\[ E[g^t + b^t - \tilde{g}^t | F_t] = 0, \]

which implies that

\[ E[X_t | F_t] = \langle E[g^t + b^t - \tilde{g}^t | F_t], x^t - x^* \rangle = 0. \]

Hence, the sequence \( \{X_t\} \) is a martingale difference sequence. Next, we estimate the probability \( P[|X_t| \geq a | F_t] \). We have the bound

\[ |X_t| = |\langle g^t + b^t - \tilde{g}^t, x^t - x^* \rangle| \leq \|g^t + b^t - \tilde{g}^t\|_1 \|x^t - x^*\|_{\infty} \leq \|g^t + b^t - \tilde{g}^t\|_1 \leq \|g^t - \tilde{g}^t\|_1 + \|b^t\|_1. \]

Since \( M \) satisfies the condition in Lemma EC.1, we know \( \|b^t\|_1 \leq \epsilon / 2T \). Recalling Assumption 3, we get \( |g^t_i| \leq L \) for all \( i \in [d] \). By the truncation rule and the assumption \( M \geq L \), we have

\[ |\tilde{g}^t_i - g^t_i| = |(\tilde{g}^t_i \wedge M) \vee (-M) - g^t_i| \leq |\tilde{g}^t - g^t| \quad \forall i \in [d]. \]

Hence, we get

\[ |X_t| \leq \frac{\epsilon}{2T} + \|\tilde{g}^t - g^t\|_1. \] (EC.3)

Define random variables \( Y_i := |\tilde{g}^t_i - g^t_i| \) for all \( i \in [d] \). By Assumption 3, \( Y_i \) is sub-Gaussian with parameter \( \sigma^2 \). Hence, we have

\[ Y := \|\tilde{g}^t - g^t\|_1 = \sum_{i=1}^{d} Y_i \]
is sub-Gaussian with parameter $d\sigma^2$. First, we consider the case when $a \geq \epsilon/T$. Using inequality (EC.3), it follows that
\[
P[|X_t| \geq a \mid \mathcal{F}_t] \leq P\left[\frac{\epsilon}{2T} + Y \geq a\right] \leq P\left[Y \geq a - \frac{\epsilon}{2T}\right] \leq P\left[Y \geq \frac{a}{2}\right] \leq 2\exp\left(-\frac{a^2}{8d\sigma^2}\right),
\] (EC.4)
where the last inequality is from Hoeffding bound. In this case, we know condition (7) holds with
\[
b_1 = 1, \quad b_2 = \frac{1}{8d\sigma^2}.
\]
Now, we consider the case when $a < \epsilon/T$. In this case, by the assumption that $T \geq 2\epsilon/\sigma$, we have
\[
2b_1 \exp\left(-b_2 a^2\right) > 2\exp\left(-\frac{1}{8d\sigma^2} \cdot \frac{\epsilon^2}{T^2}\right) \geq 2\exp\left(-\frac{1}{32d}\right) \geq 2\exp\left(-\frac{1}{32}\right) > 1.
\]
Hence, it holds
\[
P[|X_t| \geq a \mid \mathcal{F}_t] \leq 1 < 2b_1 \exp\left(-b_2 a^2\right).
\]
Combining with inequality (EC.4), we know condition (7) holds with $b$ and $c$ defined above. Using Lemma 3, we know
\[
\frac{1}{T} \sum_{t=0}^{T-1} X_t \leq \sqrt{\frac{224d\sigma^2}{T} \log\left(\frac{1}{\delta}\right)}
\]
holds with probability at least $1 - \delta$. \qed

Then, we prove a lemma similar to the Lemma in Zinkevich (2003).

**Lemma EC.3.** Suppose Assumptions 1-5 hold and let $x^*$ be a minimizer of $f(x)$. If we choose
\[
\eta = \frac{1}{M \sqrt{T}},
\]
then we have
\[
\frac{1}{T} \sum_{t=0}^{T-1} \langle \tilde{g}^t, x^t - x^* \rangle \leq \frac{dM}{\sqrt{T}}
\]

**Proof.** We define $\tilde{x}^{t+1} := x^t - \eta \tilde{g}^t$ as the next point before the projection onto $[0,1]^d$. Recalling the non-expansion property of orthogonal projection, we get
\[
||x^{t+1} - x^*||_2^2 = ||\mathcal{P}(\tilde{x}^{t+1} - x^*)||_2^2 \leq ||\tilde{x}^{t+1} - x^*||_2^2 = ||x^t - x^* - \eta \tilde{g}^t||_2^2 \\
= ||x^t - x^*||_2^2 + \eta^2 ||\tilde{g}^t||_2^2 - 2\eta \langle \tilde{g}^t, x^t - x^* \rangle,
\]
and equivalently,
\[
\langle \tilde{g}^t, x^t - x^* \rangle = \frac{1}{2\eta} \left[ \|x^t - x^*\|_2^2 - \|x^{t+1} - x^*\|_2^2 \right] + \frac{\eta}{2} \cdot \|\tilde{g}^t\|_2^2.
\]

Summing over \( t = 0, 1, \ldots, T - 1 \), we have
\[
\sum_{t=0}^{T-1} \langle \tilde{g}^t, x^t - x^* \rangle = \frac{\|x^0 - x^*\|_2^2}{2\eta} + \frac{\eta}{2} \sum_{t=0}^{T-1} \|\tilde{g}^t\|_2^2 
\leq \frac{d \|x^0 - x^*\|_2^2}{2\eta} + \frac{\eta}{2} \sum_{t=0}^{T-1} \|\tilde{g}^t\|_2^2 \leq \frac{d}{2\eta} + \frac{\eta T d M^2}{2} = dM \sqrt{T}.
\]

By the definition of truncation, it follows that \( \|\tilde{g}\|_2^2 \leq dM^2 \). Choosing
\[
\eta := \frac{1}{M \sqrt{T}},
\]
it follows that
\[
\sum_{t=0}^{T-1} \langle \tilde{g}^t, x^t - x^* \rangle \leq \frac{d}{2\eta} + \frac{\eta}{2} \sum_{t=0}^{T-1} \|\tilde{g}^t\|_2^2 \leq \frac{d}{2\eta} + \frac{\eta T d M^2}{2} = dM \sqrt{T}.
\]

Finally, using Lemmas \[\text{EC.1}, \text{EC.2} \text{and EC.3}\] we can finish the proof of Theorem 2.

**Proof of Theorem 2.** Denote \( f^* \) as the optimal value of \( \tilde{f}(x) \). Using the convexity of \( \tilde{f}(x) \), we know
\[
\tilde{f}(\bar{x}) - f^* \leq \frac{1}{T} \sum_{t=0}^{T-1} [\tilde{f}(x^t) - f^*] \leq \frac{1}{T} \sum_{t=0}^{T-1} \langle g^t, x^t - x^* \rangle = \frac{1}{T} \sum_{t=0}^{T-1} \left[ \langle g^t, x^t - x^* \rangle + \langle \bar{g}^t, x^t - x^* \rangle - \langle b^t, x^t - x^* \rangle \right].
\]

We choose
\[
T := \frac{3584 d \sigma^2}{\epsilon^2 \log \left( \frac{2}{\delta} \right)} = \Theta \left[ \frac{d}{\epsilon^2 \log \left( \frac{1}{\delta} \right)} \right].
\]

Recalling Assumption 3, we know \( \delta \) is small enough and therefore we have the following estimates:
\[
L^2 \leq M^2 = \tilde{O} \left[ \log \left( \frac{d T}{\epsilon} \right) \right] = \tilde{O} \left[ \log \left( \frac{d^2}{\epsilon^2} \right) + \log \log \left( \frac{1}{\delta} \right) \right] \leq \frac{\epsilon^2 T}{64 d^2}, \quad T \geq \max \left\{ \frac{2\epsilon}{\sigma}, 4 \right\}.
\]
Hence, the conditions in Lemmas EC.1 and EC.2 are satisfied. By Lemma EC.1, we know
\[ -\frac{1}{T} \sum_{t=0}^{T-1} \langle b^t, x^t - x^* \rangle \leq \frac{1}{T} \sum_{t=0}^{T-1} \|b^t\|_1 \|x^t - x^*\|_\infty \leq \frac{\epsilon}{2T} \leq \frac{\epsilon}{8}. \]  
(EC.6)

By Lemma EC.2 it holds
\[ \frac{1}{T} \sum_{t=0}^{T-1} \langle g^t + b^t - \tilde{g}^t, x^t - x^* \rangle \leq \sqrt{\frac{224d\sigma^2}{T}} \log\left(\frac{2}{\delta}\right) \leq \frac{\epsilon}{4}. \]  
(EC.7)

with probability at least \(1 - \delta\), where the last inequality is from our choice of \(T\). By Lemma EC.3, we know
\[ \frac{1}{T} \sum_{t=0}^{T-1} \langle \tilde{g}^t, x^t - x^* \rangle \leq \frac{dM}{\sqrt{T}} \leq \frac{\epsilon}{8}. \]  
(EC.8)

Substituting inequalities (EC.6), (EC.7) and (EC.8) into inequality (EC.5), we get
\[ \tilde{f}(\bar{x}) - f^* \leq \frac{\epsilon}{2} \]
holds with probability at least \(1 - \delta/2\). By the results of Theorem 1 we know Algorithm 2 returns an \((\epsilon, \delta)\)-PGS solution.

Finally, we estimate the simulation cost of Algorithm 2. For each iteration, we need to generate a stochastic subgradient using (4) and the simulation cost is \(2d\). Hence, the total simulation cost of all iterations is
\[ 2d \cdot T = \tilde{\Theta} \left[ \frac{d^2}{\epsilon^2} \log\left(\frac{1}{\delta}\right) \right]. \]

By Theorem 1 the simulation cost of rounding process is at most
\[ O \left[ \frac{d}{\epsilon^2} \log\left(\frac{1}{\delta}\right) \right]. \]

Thus, we know the total simulation cost of Algorithm 2 is at most
\[ \tilde{O} \left[ \frac{d^2}{\epsilon^2} \log\left(\frac{1}{\delta}\right) \right]. \]
### EC.1.3. Proof of Theorem 3

The proof follows a similar way as Theorem 2. We first bound the noise term by Azuma’s inequality.

**Lemma EC.4.** Suppose Assumptions 1-6 hold and let \( x^* \) be a minimizer of \( f(x) \). Then, it holds

\[
\frac{1}{T} \sum_{t=0}^{T-1} \langle g^t - \hat{g}^t, x^t - x^* \rangle \leq \left( \frac{3L}{2} + G \right) \sqrt{\frac{2}{T} \log\left( \frac{1}{\delta} \right)}
\]

with probability at least \( 1 - \delta \).

**Proof.** Same as the proof of Lemma EC.2, the fact that \( \hat{g}^t \) is unbiased implies that

\[
X_t := \langle g^t - \hat{g}^t, x^t - x^* \rangle \quad t = 0, 1, \ldots, T - 1
\]

is a martingale difference sequence. By Assumption 6 and property (v) in Lemma 2, we know

\[
|X_t| = |\langle g^t - \hat{g}^t, x^t - x^* \rangle| \leq \|g^t - \hat{g}^t\|_1 \|x^t - x^*\|_\infty \leq \|g^t - \hat{g}^t\|_1 \leq 3L/2 + G,
\]

which implies that the condition (11) holds with \( b = 3L/2 + G \). Using Lemma 4, we get the conclusion of this lemma. \( \square \)

The following lemma bounds the error of the algorithm and is similar to Theorem 3.2.2 in Nesterov (2018).

**Lemma EC.5.** Suppose Assumptions 1-6 hold and let \( x^* \) be a minimizer of \( f(x) \). If we choose

\[
\eta = \sqrt{\frac{d}{TG^2}},
\]

then we have

\[
\frac{1}{T} \sum_{t=0}^{T-1} \langle \hat{g}^t, x^t - x^* \rangle \leq \sqrt{\frac{dG^2}{T}}.
\]

**Proof.** We define \( \tilde{x}^{t+1} := x^t - \eta \hat{g}^t \) as the next point before the projection onto \([0,1]^d\). Recalling the non-expansion property of orthogonal projection, we get

\[
\|x^{t+1} - x^*\|_2^2 = \|P(\tilde{x}^{t+1} - x^*)\|_2^2 \leq \|\tilde{x}^{t+1} - x^*\|_2^2 = \|x^t - x^* - \eta \hat{g}^t\|_2^2
\]

\[
= \|x^t - x^*\|_2^2 + \eta^2 \|\hat{g}^t\|_2^2 - 2\eta \langle \hat{g}^t, x^t - x^* \rangle,
\]

where \( P \) is the orthogonal projection onto \([0,1]^d\).
and equivalently,
\[
\langle \hat{g}^t, x^t - x^* \rangle = \frac{1}{2\eta} \left[ \left\| x^t - x^* \right\|_2^2 - \left\| x^{t+1} - x^* \right\|_2^2 \right] + \frac{\eta}{2} \cdot \left\| \hat{g}^t \right\|_2^2.
\]

Using Assumption 6, we know \( \| \hat{g}^t \|_2^2 \leq \| \hat{g}^t \|_1^2 \leq G^2 \) and therefore
\[
\langle \hat{g}^t, x^t - x^* \rangle = \frac{1}{2\eta} \left[ \left\| x^t - x^* \right\|_2^2 - \left\| x^{t+1} - x^* \right\|_2^2 \right] + \frac{\eta G^2}{2}.
\]

Summing over \( t = 0, 1, \ldots, T - 1 \), we have
\[
\sum_{t=0}^{T-1} \langle \hat{g}^t, x^t - x^* \rangle = \frac{\| x^0 - x^* \|_2^2 - \| x^T - x^* \|_2^2}{ 2\eta} + T \cdot \frac{\eta G^2}{2} \leq \frac{d \| x^0 - x \|_\infty^2}{ 2\eta} + \frac{\eta T G^2}{2} \leq \frac{d}{ 2\eta} + \frac{\eta T G^2}{2}.
\]

Choosing
\[
\eta := \sqrt{\frac{d}{ TG^2}},
\]

it follows that
\[
\sum_{t=0}^{T-1} \langle \hat{g}^t, x^t - x^* \rangle \leq G\sqrt{dT}.
\]

Now, we prove Theorem 3 using Lemmas EC.4 and EC.5.

**Proof of Theorem 3.** According to the proof of Theorem 2, we have
\[
\tilde{f}(\bar{x}) - f^* = \frac{1}{T} \sum_{t=0}^{T-1} \left[ \tilde{f}(x^t) - f^* \right] \leq \frac{1}{T} \sum_{t=0}^{T-1} \langle \hat{g}^t, x^t - x^* \rangle + \frac{1}{T} \sum_{t=0}^{T-1} \langle g^t - \hat{g}^t, x^t - x^* \rangle,
\]

By Lemmas EC.4 and EC.5, it holds
\[
\frac{1}{T} \sum_{t=0}^{T-1} \langle \hat{g}^t, x^t - x^* \rangle \leq \left( \frac{3L}{2} + G \right) \sqrt{\frac{2}{T} \log\left( \frac{2}{\delta} \right)}, \quad \frac{1}{T} \sum_{t=0}^{T-1} \langle g^t - \hat{g}^t, x^t - x^* \rangle \leq \sqrt{\frac{dG^2}{T}}
\]

with probability at least \( 1 - \delta/2 \). Choosing
\[
T = \left( \frac{3L}{2} + G \right)^2 \cdot \frac{32}{\epsilon^2} \log\left( \frac{2}{\delta} \right) = \Theta\left[ \frac{(L + G)^2}{\epsilon^2} \log\left( \frac{1}{\delta} \right) \right],
\]

we know
\[
T \geq \frac{16dG^2}{\epsilon^2}.
\]
when $\delta$ is small enough. Hence, we have

\[
\frac{1}{T} \sum_{t=0}^{T-1} \langle g^t, x^t - x^* \rangle \leq \frac{\epsilon}{4}, \quad \frac{1}{T} \sum_{t=0}^{T-1} \langle \hat{g}^t, x^t - x^* \rangle \leq \frac{\epsilon}{4}
\]

holds with probability at least $1 - \delta/2$. Substituting into inequality (EC.9), we have

\[
\tilde{f}(\bar{x}) - f^* \leq \frac{\epsilon}{2}
\]

holds with probability at least $1 - \delta/2$. By the results of Theorem 1, we know Algorithm 2 returns an $(\epsilon, \delta)$-PGS solution.

Finally, we estimate the simulation cost of Algorithm 2. For each iteration, the simulation cost is decided by the generation of a stochastic subgradient, which is at most $\beta$ by Assumption 6. Hence, the total simulation cost of all iterations is

\[
O[\beta T] = \tilde{O} \left[ \frac{\beta(L + G)^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].
\]

By Theorem 1, the simulation cost of rounding process is at most

\[
O \left[ \frac{d}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].
\]

Thus, we know the total simulation cost of Algorithm 2 is at most

\[
\tilde{O} \left[ \frac{\beta(L + G)^2 + d}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].
\]

\[\square\]

**EC.2. Proofs in Section 4**

**EC.2.1. Proof of Theorem 4**

*Proof of Theorem 4.* To prove the function is well-defined, we only need to show that for any two different points $y, z \in [N - 1]^d$ such that $C_y \cap C_z \neq \emptyset$, we have $\tilde{f}_y(x) = \tilde{f}_z(x)$ for all $x \in C_y \cap C_z$. We first consider the case when $\|y - z\|_1 = 1$. Without loss of generality, we assume

\[
y = (1, 1 \ldots, 1), \quad z = (2, 1 \ldots, 1).
\]
In this case, we know that

\[ C_y \cap C_z = \{(2, x_2, \ldots, x_d) : x_2, \ldots, x_d \in [0, 1]\}. \]

Suppose point \( x \in C_y \cap C_z \). We first calculate \( \tilde{f}_y(x) \). We can define the “local coordinate” of \( x \) in \( C_y \) as

\[ x - y = (1, x_2 - 1, \ldots, x_d - 1). \]

Let \( \alpha_1 \) be a consistent permutation of \( x \) in \( C_y \) and and \( S^{1,i} \) be the corresponding \( i \)-th neighbouring point. Since \( (x - y)_1 = 1 \) is not smaller than any other components, we can assume \( \alpha_1(1) = 1 \) and calculate \( \tilde{f}_y(x) \) as

\[
\tilde{f}_y(x) = [1 - (x - y)_{\alpha_1(1)}] f(S^{1,0}) + \sum_{i=1}^{d-1} [(x - y)_{\alpha_1(i)} - (x - y)_{\alpha_1(i+1)}] f(S^{1,i}) + (x - y)_{\alpha_1(d)} f(S^{1,d})
\]

(EC.10)

\[
= \sum_{i=1}^{d-1} [(x - y)_{\alpha_1(i)} - (x - y)_{\alpha_1(i+1)}] f(S^{1,i}) + (x - y)_{\alpha_1(d)} f(S^{1,d})
\]

\[
= \sum_{i=1}^{d-1} [x_{\alpha_1(i)} - x_{\alpha_1(i+1)}] f(S^{1,i}) + [x_{\alpha_1(d)} - 1] f(S^{1,d}).
\]

Next, we consider \( \tilde{f}_z(x) \) and define the “local coordinate” of \( x \) in \( C_z \) is

\[ x - z = (0, x_2 - 1, \ldots, x_d - 1). \]

We define the permutation \( \alpha_2 \) as

\[ \alpha_2(i) = \alpha_1(i + 1) \quad \forall i \in [d - 1], \quad \alpha_2(d) = \alpha_1(1) = 1. \]

By the definition of \( \alpha_1 \), we know

\[ (x - z)_{\alpha_2(i)} = (x - y)_{\alpha_1(i + 1)} \geq (x - y)_{\alpha_1(i + 2)} = (x - z)_{\alpha_2(i + 1)} \quad \forall i \in [d - 2], \]

\[ (x - z)_{\alpha_2(d - 1)} \geq 0 = (x_z)_{\alpha_2(d)}. \]
Hence, we know \( \alpha_2 \) is a consistent permutation of \( x \) in \( C_z \) and let \( S^{2,i} \) be the corresponding \( i \)-th neighbouring point of \( x \) in \( C_z \). Similar to the first case, the Lovász extension \( \tilde{f}_y(x) \) can be calculated as

\[
\tilde{f}_y(x) = [1 - (x - z)_{\alpha_2(1)}] f(S^{2,0}) + \sum_{i=1}^{d-1} [(x - z)_{\alpha_2(i)} - (x - z)_{\alpha_2(i+1)}] f(S^{2,i}) + (x - z)_{\alpha_2(d)} f(S^{2,d})
\]

(EC.11)

Recalling the fact that \( z = y + e_1 \), for any \( i \in [d-1] \), we have

\[
S^{2,i} = z + \sum_{j=1}^{i} e_{\alpha_2(j)} = y + e_1 + \sum_{j=1}^{i} e_{\alpha_1(j+1)} = y + \sum_{j=1}^{i+1} e_{\alpha_1(i)} = S^{1,i+1}.
\]

Substituting into equation (EC.11), we know

\[
\tilde{f}_y(x) = [2 - x_{\alpha_2(1)}] f(S^{2,0}) + \sum_{i=1}^{d-1} [x_{\alpha_2(i)} - x_{\alpha_2(i+1)}] f(S^{2,i}) + f(S^{2,d-1})
\]

\[
= [2 - x_{\alpha_2(1)}] f(S^{1,1}) + \sum_{i=1}^{d-2} [x_{\alpha_2(i)} - x_{\alpha_2(i+1)}] f(S^{1,i+1}) + [x_{\alpha_2(d-1)} - x_{\alpha_2(d)}] f(S^{1,d}) + f(S^{1,d})
\]

\[
= [x_{\alpha_1(1)} - x_{\alpha_1(2)}] f(S^{1,1}) + \sum_{i=1}^{d-2} [x_{\alpha_1(i)} - x_{\alpha_1(i+2)}] f(S^{1,i+1}) + [x_{\alpha_1(d-1)} - 2] f(S^{1,d}) + f(S^{1,d})
\]

\[
= \sum_{i=1}^{d-1} [x_{\alpha_1(i)} - x_{\alpha_1(i+1)}] f(S^{1,i}) + [x_{\alpha_1(d)} - 1] f(S^{1,d}),
\]

which is equal to \( \tilde{f}_y(x) \) by equation (EC.10).

Then, we consider the case when \( \|y - z\|_1 > 1 \). Since \( C_y \cap C_z \neq \emptyset \), we know \( \|y - z\|_\infty = 1 \). Without loss of generality, we consider the case when

\[
y = (1, 1, \ldots, 1), \quad z = y + \sum_{j=1}^{k} e_j,
\]

where constant \( k \in [d] \). In this case, we know

\[
C_y \cap C_z = \{ x \in \mathbb{R}^d : x_j = 2, \forall j \leq k; x_j \in [0, 1], \forall j \geq k + 1 \}.
\]
We define
\[ y_i := y + \sum_{j=1}^{i} e_j \quad \forall i \in \{0, 1, \ldots, k\}. \]

Then, it follows that
\[ \|y_i - y_{i-1}\|_1 = 1 \quad \forall i \in [k], \quad y_0 = y, \quad y_k = z \]

and
\[ x \in C_y \cap Z \subset C_{y_i} \cap C_{y_{i-1}} = \{ x \in \mathbb{R}^d : x_i = 2, \ x_j \in [0, 1], \ \forall j \in [d]\setminus\{i\} \} \quad \forall i \in [k]. \]

Hence, by the results for the case when \( \|y - z\|_1 = 1 \), we know
\[ \tilde{f}_y(x) = \tilde{f}_{y_0}(x) = \tilde{f}_{y_1}(x) = \cdots = \tilde{f}_{y_k}(x) = \tilde{f}_z(x), \]

which means \( \tilde{f}(x) \) is well-defined.

Finally, we prove the convexity of \( \tilde{f}(x) \). Since the Lovász extension is the support function of submodular functions (Fujishige 2005, section 6.3), the function \( \tilde{f}_y(x) \) is the support function of \( f(x) \) inside cube \( C_y \). In addition, Theorem 7.20 in Murota (2003) implies that the \( L^2 \)-convex function \( f(x) \) is integrally convex. Hence, we know that the support function of \( f(x) \) on \( X \) is equal to \( \tilde{f}_y(x) \) in each cube \( C_y \). By the definition of \( \tilde{f}(x) \) in (12), the function \( \tilde{f}(x) \) is the support function of \( f(x) \) on \( X \). Since support functions are convex, we know \( \tilde{f}(x) \) is convex. \( \square \)

**EC.2.2. Proof of Theorem 5**

**Proof of Theorem 5** The proof can be done in the same way as Theorem 2 and we only give a sketch of the proof. We use the same notation as the proof of Theorem EC.1.

- If we have
  \[ M \geq 2\sigma \cdot \sqrt{\frac{4\sigma dNT}{\epsilon}} = \tilde{\Theta}\left(\sqrt{\frac{dNT}{\epsilon}}\right), \quad T \geq \frac{2\epsilon}{\sigma}, \]
  then the proof of Lemma EC.1 implies that
  \[ \|b^t\|_1 \leq \frac{\epsilon}{2T} \quad \forall t \in \{0, 1, \ldots, T - 1\}. \]
• If we have
\[
M = \max \left\{ L, 2\sigma \cdot \sqrt{\log \left( \frac{4dNT}{\epsilon} \right)} \right\} = \tilde{\Theta} \left[ \sqrt{\log \left( \frac{dNT}{\epsilon} \right)} \right], \quad T \geq \frac{2N\epsilon}{\sigma},
\]
then the proof of Lemma [EC.2] shows that
\[
\frac{1}{T} \sum_{t=0}^{T-1} X_t \leq \sqrt{\frac{224dN^2\sigma^2}{T} \log \left( \frac{1}{\delta} \right)}
\]
holds with probability at least 1 − δ.

• If we choose
\[
\eta = \frac{N}{d\sqrt{M}},
\]
then the proof of Lemma [EC.3] implies that
\[
\frac{1}{T} \sum_{t=0}^{T-1} \langle \tilde{g}_t, x_t - x^* \rangle \leq \frac{dNM}{\sqrt{T}}.
\]
Hence, choosing
\[
T = \tilde{\Theta} \left[ \frac{dN^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right], \quad M = \tilde{\Theta} \left[ \sqrt{\log \left( \frac{dNT}{\epsilon} \right)} \right], \quad \eta = \frac{N}{M\sqrt{T}}
\]
and using the inequality [EC.5], we know the averaging point \( \bar{x} \) is an \((\epsilon/2, \delta/2)\)-PGS solution. Combining with Theorem 1, Algorithm 2 returns an \((\epsilon, \delta)\)-PGS solution. Since the simulation cost of each iteration is 2\(d\), the total simulation cost of Algorithm 2 is at most
\[
\tilde{O} \left[ \frac{d^2N^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right] + O \left[ \frac{d}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right] = \tilde{O} \left[ \frac{d^2N^2}{\epsilon^2} \log \left( \frac{1}{\delta} \right) \right].
\]
\[\square\]

**EC.2.3. Proof of Theorem 7**

**Proof of Theorem 7.** We first prove the sufficiency part and then consider the necessity part.

**Sufficiency.** Suppose there exists a constant \( \eta > 0 \) such that the function \( \tilde{f}(x) \) satisfies the WSM condition with \( \eta \). Considering any point \( x \in X \setminus \{ x^* \} \), we know \( \| x - x^* \|_\infty \geq 1 \) and, by the WSM condition,
\[
f(x) - f^* = \tilde{f}(x) - f^* \geq \eta^{-1} \| x - x^* \|_\infty \geq \eta^{-1}.
\]
Thus, we know the indifference zone parameter for \( f(x) \) is at least \( \eta^{-1} \) and \( f(x) \in MC_{\eta^{-1}} \).
Necessity. Suppose there exists a constant \( c > 0 \) such that
\[
f(x) - f^* \geq c \quad \forall x \in \mathcal{X}\setminus\{x^*\}.
\]
We first consider point \( x \in [1, N]^d \) such that \( \|x - x^*\|_\infty \leq 1 \). In this case, we know there exists a cube \( C_y \) containing both \( x \) and \( x^* \). By the definition of Lovász extension, we know that
\[
\tilde{f}(x) = [1 - x_{\alpha_x(1)}] f(S^{x,0}) + \sum_{i=1}^{d-1} [x_{\alpha_x(i)} - x_{\alpha_x(i+1)}] f(S^{x,i}) + x_{\alpha_x(d)} f(S^{x,d}) = \sum_{i=0}^{d} \lambda_i f(S^{x,i}),
\]
where we define
\[
\lambda_i := x_{\alpha_x(i)} - x_{\alpha_x(i+1)} \quad \forall i \in [d-1], \quad \lambda_0 := 1 - x_{\alpha_x(1)}, \quad \lambda_d := x_{\alpha_x(d)}.
\]
Recalling the definition of consistent permutation, we get
\[
\sum_{i=0}^{d} \lambda_i = 1, \quad \lambda_i \geq 0 \quad \forall i \in \{0, \ldots, d\}
\]
and \( \tilde{f}(x) \) is a convex combination of \( f(S^{x,0}), \ldots, f(S^{x,d}) \). In addition, we can calculate that
\[
\left( \sum_{i=0}^{d} \lambda_i S^{x,i}_{\alpha_x(k)} \right)_{\alpha_x(k)} = \sum_{i=0}^{d} \lambda_i S^{x,i}_{\alpha_x(k)} = \sum_{i=0}^{d} \lambda_i \cdot 1(i \leq k) = \sum_{i=k}^{d} \lambda_i = x_{\alpha_x(k)},
\]
which implies that
\[
x = \sum_{i=0}^{d} \lambda_i S^{x,i}_{\alpha_x(k)}.
\]
If \( x^* \notin \{S^{x,0}, \ldots, S^{x,d}\} \), the assumption that indifference zone parameter is \( c \) gives
\[
\tilde{f}(x) - f^* = \sum_{i=0}^{d} \lambda_i [f(S^{x,i}) - f^*] \geq \sum_{i=0}^{d} \lambda_i \cdot c = c.
\]
Combining with \( \|x - x^*\|_\infty \leq 1 \), we have
\[
\|x - x^*\|_\infty \leq c^{-1} \cdot \left[ \tilde{f}(x) - f^* \right].
\]
Otherwise if \( x^* = S^{x,i} \) for some \( i \in \{0, \ldots, d\} \). Then, we know
\[
\tilde{f}(x) - f^* = \sum_{i=0}^{d} \lambda_i [f(S^{x,i}) - f^*] \geq \sum_{i \neq k} \lambda_i \cdot c = (1 - \lambda_k)c
\]
and
\[ \|x - x^*\|_\infty = \left\| \sum_{i=0}^{d} \lambda_i S^{x,i} - x^* \right\|_\infty = \left\| \sum_{i=0}^{d} \lambda_i (S^{x,i} - x^*) \right\|_\infty = \left\| \sum_{i\neq k} \lambda_i (S^{x,i} - x^*) \right\|_\infty \leq \sum_{i\neq k} \lambda_i \|S^{x,i} - x^*\|_\infty \leq \sum_{i\neq k} \lambda_i = 1 - \lambda_k, \]
where the last inequality is because \( S^{x,i} \) and \( x^* \) are in the same cube \( C_y \). Combining the above two inequalities, it follows that
\[ \|x - x^*\|_2 \leq c^{-1} \cdot \left[ \tilde{f}(x) - f^* \right], \]
which means that the WSM condition holds with \( \eta = c^{-1} \). Now we consider point \( x \in [1, N]^d \) such that \( \|x - x^*\|_\infty \geq 1 \). We define
\[ \tilde{x} := x^* + \frac{x - x^*}{\|x - x^*\|_\infty} \]
to be the point on the segment \( xx^* \) such that \( \|\tilde{x} - x^*\|_\infty = 1 \). By the convexity of \( \tilde{f}(x) \) and the WSM condition for point \( \tilde{x} \), we know
\[ \tilde{f}(x) - f^* \geq \frac{\|x - x^*\|_\infty}{\|\tilde{x} - x^*\|_\infty} \left[ \tilde{f}(\tilde{x}) - f^* \right] = \frac{\tilde{f}(\tilde{x}) - f^*}{\|\tilde{x} - x^*\|_\infty} \cdot \|x - x^*\|_\infty \geq c^{-1} \cdot \|x - x^*\|_\infty, \]
which shows that the WSM condition holds with \( \eta = c^{-1} \). Hence, the WSM condition holds for all points in \([1, N]^d\) with \( \eta = c^{-1} \).

**EC.2.4. Proof of Theorem 8**

**Proof of Theorem 8**  We first prove the correctness of Algorithm 3. Let \( x^* \) be the minimizer of \( f(x) \) and \( f^* := f(x^*) \). We use the induction method to prove that, for each epoch \( e \), it holds
\[ \tilde{f}(x_e) - f^* \leq \epsilon_e \]
with probability at least \( 1 - (e + 1)\delta/(2E) \). For epoch 0, the solution \( x_0 \) is \((\epsilon_0, \delta/(2E))\)-PGS and we know
\[ \tilde{f}(x_0) - f^* \leq \epsilon_0 \]
holds with probability at least \( 1 - \delta/(2E) \). We assume that the above event happens for the \((e - 1)\)th epoch with probability at least \( 1 - e \cdot \delta/(2E) \) and consider the case when this event happens.
By Theorem 7, function $\tilde{f}(x)$ satisfies the WSM condition with $\eta = c^{-1}$. Hence, the intermediate solution $x_{e-1}$ satisfies

$$\|x_{e-1} - x^*\|_\infty \leq c^{-1} \left[ \tilde{f}(x_{e-1}) - f^* \right] \leq c^{-1} \epsilon_{e-1} = c^{-1} \cdot 2^{-c+1} \epsilon_0 = 2^{-c-1} N,$$

which implies that $x^* \in \mathcal{N}(x_{e-1}, 2^{-c-1} N) = \mathcal{N}_c$ and therefore $x^* \in \mathcal{N}_c$. For the epoch $e$, it holds

$$\tilde{f}(x_e) - f^* \leq \tilde{f}(x_e) - \min_{x \in \mathcal{N}_c} \tilde{f}(x) \leq \epsilon_e$$

with probability at least $1 - \delta/(2E)$. Hence, the above event happens with probability at least $1 - \delta/(2E) - e \cdot \delta/(2E) = 1 - (e + 1)\delta/(2E)$ for epoch $e$. By the induction method, we know the claim holds for all epochs. Considering the last epoch, we know

$$\tilde{f}(x_{E-1}) - f^* \leq \epsilon_{E-1} = 2^{-E+1} \epsilon_0 = 2^{-\lfloor \log_2(N) \rfloor - 2} \cdot cN \leq 2^{-\log_2(N) - 2} \cdot cN = c/4$$

holds with probability at least $1 - \delta/2$. Thus, we know $x_{E-1}$ satisfies the $(c/4, \delta/2)$-PGS guarantee. By Theorem 1, the integral solution returned by Algorithm 3 satisfies the $(c/2, \delta)$-PGS guarantee. Since the indifference zone parameter is $c$, the solution satisfying the $(c/2, \delta)$-PGS guarantee must satisfies the $(c, \delta)$-PCS-IZ guarantee.

Next, we estimate the asymptotic simulation cost of Algorithm 3. By Theorem 2, the simulation cost of epoch $e$ is at most

$$\tilde{O} \left[ \frac{d^2 (2^{-c} N)^2}{c^2} \log\left( \frac{E}{\delta} \right) \right] = \tilde{O} \left[ \frac{d^2 (2^{-c} N)^2}{(2^{-c-2} \cdot cN)^2} \log\left( \frac{E}{\delta} \right) \right] = \tilde{O} \left[ \frac{d^2 \log(1/\delta)}{c^2} \right].$$

Summing over $e = 0, 1, \ldots, E - 1$, we know the total simulation cost of $E$ epochs is at most

$$\tilde{O} \left[ E \cdot \frac{d^2 \log(1/\delta)}{c^2} \right] = \tilde{O} \left[ \frac{d^2 \log(N)}{c^2} \log(1/\delta) \right].$$

By Theorem 1, the simulation cost of the rounding process is at most

$$O \left[ \frac{d}{c^2} \log\left( \frac{1}{\delta} \right) \right].$$

Combining the two parts, we know the asymptotic simulation cost of Algorithm 3 is at most

$$\tilde{O} \left[ \frac{d^2 \log(N)}{c^2} \log\left( \frac{1}{\delta} \right) \right].$$
**EC.3. Proofs in Section 5**

**EC.3.1. Proof of Theorem 10**

*Proof of Theorem 10.* In this proof, we change the feasible set to $\mathcal{X} = \{0, 1, \ldots, N\}^d$, where $N \geq 1$. We split the proof into three steps.

**Step 1.** We first show that the construction of $L^2$-convex functions can be reduced to the construction of submodular functions. Equivalently, we show that any submodular function defined on $\{0, 1\}^d$ can be extended to a $L^2$-convex function on $\mathcal{X}$ with the same convex extension after scaling. Let $g(x)$ be a submodular function defined on $\{0, 1\}^d$ and $\tilde{g}(x)$ be the Lovász extension of $g(x)$. We first extend the domain of the Lovász extension to $[0, N]^d$ by scaling, i.e.,

$$
\tilde{f}(x) := \tilde{g}(x/N) \quad \forall x \in [0, N]^d.
$$

Then, we define the discretization of $\tilde{f}(x)$ by restricting to the integer lattice

$$
f(x) := \tilde{f}(x) \quad \forall x \in \mathcal{X}.
$$

We prove that $f(x)$ is a $L^2$-convex function. By Proposition 7.25 in [Murota, 2003](#Murota2003), we know the Lovász extension $\tilde{g}(x)$ is a polyhedral $L$-convex function. Since the scaling operation does not change the $L$-convexity, we know $\tilde{f}(x)$ is also polyhedral $L$-convex. Hence, by Theorem 7.29 in [Murota, 2003](#Murota2003), the function $\tilde{f}(x)$ satisfies the SBF$^2[\mathbb{R}]$ property, namely,

$$
\tilde{f}(p) + \tilde{f}(q) \geq \tilde{f}[(p - \alpha \mathbf{1}) \lor q] + \tilde{f}(p \land (q + \alpha \mathbf{1})) \quad \forall p, q \in [0, N]^d, \alpha \geq 0.
$$

Restricting to the integer lattice, we know the SBF$^2[\mathbb{Z}]$ property holds for $f(x)$, namely,

$$
f(p) + f(q) \geq f[(p - \alpha \mathbf{1}) \lor q] + f(p \land (q + \alpha \mathbf{1})) \quad \forall p, q \in \{0, \ldots, N\}^d, \alpha \in \mathbb{N}.
$$

Finally, Theorem 7.7 in [Murota, 2003](#Murota2003) shows that the $L^2$-convexity is equivalent to the SBF$^2[\mathbb{Z}]$ property and therefore we know that $f(x)$ is a $L^2$-convex function.
Step 2. Next, we construct \( d + 1 \) submodular functions on \( \{0, 1\}^d \) and extend them to \( \mathcal{X} \) by the process defined in Step 1. The construction is based on the family of submodular functions defined in Graur et al. (2020). We denote \( \mathcal{I} := \{0\} \cup [d] \). For each \( i \in \mathcal{I} \), we define point \( x^i \in \{0, 1\}^d \) as

\[
x^i := \sum_{j=1}^i e_j,
\]

where \( e_j \) is the \( j \)-th unit vector of \( \mathbb{R}^d \). Index \( j(x) \) is defined as the maximal index \( j \) such that \( x^i = 1 \) \( \forall i \in [j] \).

If \( x_1 = 0 \), then we define \( j(x) = 0 \). Given \( c : \mathcal{I} \mapsto \mathbb{R} \), we define a function on \( \{0, 1\}^d \) as

\[
g^c(x) := \begin{cases} -c(i) & \text{if } x = x^i \text{ for some } i \in \mathcal{I} \\ (\|x\|_1 - j(x)) \cdot (d + 2 - \|x\|_1) & \text{otherwise}. \end{cases}
\]

By Lemma 6 in Graur et al. (2020), the function \( g^c(x) \) is submodular if \( c(\mathcal{I}) \subset \{0, 1\} \). Using the fact that convex combinations of submodular functions are still submodular, we know that \( g^c(x) \) is submodular for any \( c \) such that \( c(\mathcal{I}) \subset [0, 1] \). Then, for each \( i \in \mathcal{I} \), we construct

\[
c^i(0) := \frac{1}{2}, \quad c^i(j) := \begin{cases} 1 & j = i \\ 0 & j \neq i \end{cases} \quad \forall j \in [d].
\]

We denote \( g^i(x) := g^{c^i}(x) \) and let \( f^i(x) \) be the extension of \( 6\varepsilon \cdot g^i(x) \) on \( \mathcal{X} \) by the process in Step 1. By the result in Step 1, we know that \( f^i(x) \) is \( L^3 \)-convex.

Next, we prove that \( f^0(x) \) has disjoint set of \( \varepsilon \)-optimal solutions with \( f^i(x) \) for any \( i \in [d] \). For each \( f^i(x) \), we define the set of \( \varepsilon \)-optimal solutions as

\[
\mathcal{X}_i^\varepsilon := \{x \in \mathcal{X} : f^i(x) - \min_y f^i(y) \leq \varepsilon\}.
\]

We first consider \( \mathcal{X}_i^0 \). By the definition of \( g^0(x) \), we know that

\[
f^0(x^0) = g^0(x^0) = -3\varepsilon, \quad f^0(x) = g^0(x/N) \geq 0 \quad \forall x \in \{0, N\}^d \setminus \{x^0\},
\]

(EC.12)
which implies that

\[ \mathcal{X}_\epsilon^0 = \{ x \in \mathcal{X} : f^0(x) \leq -2\epsilon \}. \]

Since \( f^0(x) \) is defined by the scaled Lovász extension of \( g^0(x) \), we have

\[ f^0(x) = N^{-1} \cdot \left[ (N - x_{\alpha(1)}) f^0(S^0) + \sum_{i=1}^{d-1} (x_{\alpha(i)} - x_{\alpha(i+1)}) f^0(S^i) + x_{\alpha(d)} f^0(S^d) \right], \quad \text{(EC.13)} \]

where \( \alpha \) is a consistent permutation of \( x/N \) and \( S^i := N \cdot S^i/N, i \in \{0, N\}^d \) is the \( i \)-th neighbouring points of \( x \) in the cube \( \{0, N\}^d \). Using the relation in (EC.12) and the fact \( S^0 = x^0 \), we get

\[ f^0(x) \geq N^{-1} \cdot (N - x_{\alpha(1)}) f(S_0) = N^{-1} \cdot (N - x_{\alpha(1)}) f(x^0) = -3\epsilon N^{-1} \cdot (N - x_{\alpha(1)}). \]

Hence, for any point \( x \in \mathcal{X}_\epsilon^0 \), we have \( N - x_{\alpha(1)} = N - \max_i x_i \geq 2N/3 \) and therefore

\[ \mathcal{X}_\epsilon^0 \subset \{ x \in \mathcal{X} : N - \max_i x_i \geq 2N/3 \} = \{ x \in \mathcal{X} : \max_i x_i \leq N/3 \}. \quad \text{(EC.14)} \]

Next, we consider \( \mathcal{X}_\epsilon^i \) with \( i \in [d] \). By the definition of \( g^i(x) \), we have

\[ f^i(x^0) = g^i(x^0) = -3\epsilon, \quad f^i(x) = g^i(x) \geq -6\epsilon \ \forall x \in \{0, N\}^d \setminus \{x^0\}, \]

which implies that

\[ \mathcal{X}_\epsilon^i = \{ x \in \mathcal{X} : f^i(x) \leq -5\epsilon \}. \]

Since the consistent permutation and neighboring points only depend on the coordinate of \( x \), we know

\[ f^i(x) = N^{-1} \cdot \left[ (N - x_{\alpha(1)}) f^i(S^0) + \sum_{i=1}^{d-1} (x_{\alpha(i)} - x_{\alpha(i+1)}) f^i(S^i) + x_{\alpha(d)} f^i(S^d) \right] \]

\[ \geq N^{-1} \cdot \left[ -3\epsilon (N - x_{\alpha(1)}) - 6\epsilon \sum_{i=1}^{d-1} (x_{\alpha(i)} - x_{\alpha(i+1)}) - 6\epsilon \cdot x_{\alpha(d)} \right] \]

\[ = N^{-1} \cdot \left[ -3\epsilon (N - x_{\alpha(1)}) - 6\epsilon \cdot x_{\alpha(1)} \right] = -3\epsilon N^{-1} \cdot (N + x_{\alpha(1)}). \]

Hence, the set \( \mathcal{X}_\epsilon^i \) satisfies

\[ \mathcal{X}_\epsilon^i \subset \{ x \in \mathcal{X} : N + \max_i x_i \geq 5N/3 \} = \{ x \in \mathcal{X} : \max_i x_i \geq 2N/3 \}. \quad \text{(EC.16)} \]

Combining the relations (EC.14) and (EC.16), we know \( \mathcal{X}_\epsilon^0 \cap \mathcal{X}_\epsilon^i = \emptyset \) for all \( i \in [d] \).
Step 3. Finally, we give a lower bound of $T_0(\epsilon, \delta, \mathcal{MC})$. For each $i \in I$, we define $M_i$ as the model such that the objective function is $f^i(x)$ and the distribution at each point is Gaussian with variance $\sigma^2$. Same as the one-dimensional case, given a zeroth-order algorithm and an model $M$, we denote $N_x(\tau)$ as the number of times that $F(x, \xi)$ is simulated when the algorithm terminates. By definition, we have

$$
\mathbb{E}_M[\tau] = \sum_{x \in X} \mathbb{E}_M[N_x(\tau)],
$$

where $\mathbb{E}_M$ is the expectation when the model $M$ is given. Similarly, we can define $\mathbb{P}_M$ as the probability when the model $M$ is given. Suppose $A$ is an $[(\epsilon, \delta)-\text{PGS}, \mathcal{MC}]$-algorithm and let $E$ be the event that the solution returned by $A$ is in the set $X^0_\epsilon$. Since $X^0_\epsilon \cap X_i^0 = \emptyset$ for all $i \in [d]$, we know

$$
\mathbb{P}_M[E_0] \geq 1 - \delta, \quad \mathbb{P}_M[E_i] \leq \delta \quad \forall i \in [d].
$$

Using the information-theoretical inequality (14), it holds

$$
\sum_{x \in X} \mathbb{E}_M_0[N_x(\tau)] \text{KL}(\nu_{0,x}, \nu_{i,x}) \geq d(\mathbb{P}_M_0(E), \mathbb{P}_M_i(E)) \geq d(1 - \delta, \delta) \geq \log\left(\frac{1}{2 \cdot 2 \delta}\right), \quad (\text{EC.17})
$$

where $d(x, y) := x \log(x/y) + (1 - x) \log((1 - x)/(1 - y))$, $\text{KL}(\cdot, \cdot)$ is the KL divergence and $\nu_{i,x}$ is the distribution of $F^i(x, \xi)$. Since the distributions $\nu_{i,x}$ are Gaussian with variance $\sigma^2$, the KL divergence can be calculated as

$$
\text{KL}(\nu_{0,x}, \nu_{i,x}) = 2\sigma^{-2} \left(f^0(x) - f^i(x)\right)^2.
$$

Now we estimate $f^0(x) - f^i(x)$ for all $i \in [d]$. By equations (EC.13) and (EC.15), we get

$$
f^0(x) - f^i(x) = N^{-1} \left[ (N - x_{\alpha(1)}) \left(f^0(S^0) - f^i(S^0)\right) \right.
\left. + \sum_{j=1}^{d-1} (x_{\alpha(j)} - x_{\alpha(j+1)}) \left(f^0(S^j) - f^i(S^j)\right) + x_{\alpha(d)} \left(f^0(S^d) - f^i(S^d)\right) \right],
$$

where $\alpha$ is a consistent permutation of $x/N$ and $S^i$ is the $i$-th neighboring point of $x$ in cube $\{0, N\}^d$. By the definition of $f^0(x)$ and $f^i(x)$, we have

$$
f^0(x) - f^i(x) = \begin{cases} 6\epsilon & \text{if } x = x^i \\ 0 & \text{otherwise.} \end{cases}
$$
Since $\|x^i\|_1 = i$ and $\|S^j\|_1 = j$ for all $j \in \mathcal{I}$, we know

$$f^0(S^i) - f^i(S^i) \leq 6\varepsilon, \quad f^0(S^i) - f^i(S^i) = 0 \quad \forall j \in \mathcal{I}\setminus\{i\}.$$ 

Substituting into equation (EC.18), it follows that

$$f^0(x) - f^i(x) \leq \begin{cases} 
(6\varepsilon \cdot (x_{\alpha(i)} - x_{\alpha(i+1)}))^2 & \text{if } i \in [d-1] \\
(6\varepsilon \cdot x_{\alpha(d)})^2 & \text{if } i = d.
\end{cases}$$

Hence, the KL divergence is bounded by

$$KL(\nu_0, x, \nu_i) = 2\sigma^{-2} (f^0(x) - f^i(x))^2 \leq \begin{cases} 
72\sigma^{-2} N^{-2} \varepsilon^2 \left((x_{\alpha(i)} - x_{\alpha(i+1)})^2 & \text{if } i \in [d-1] \\
72\sigma^{-2} N^{-2} \varepsilon^2 x_{\alpha(d)}^2 & \text{if } i = d.
\end{cases}$$

Substituting the KL divergence into inequality (EC.17) and summing over $i = 1, \ldots, d$, we get

$$\sum_{x \in \mathcal{X}} E_{M_0} [N_x(\tau)] \cdot 72\sigma^{-2} N^{-2} \varepsilon^2 \left(\sum_{i=1}^{d-1} (x_{\alpha(i)} - x_{\alpha(i+1)})^2 + x_{\alpha(d)}^2\right) \geq d \log \left(\frac{1}{2.4\delta}\right). \quad (EC.19)$$

Since $\alpha$ is the consistent permutation of $x$, we know

$$0 \leq x_{\alpha(i)} - x_{\alpha(i+1)} \leq N \quad \forall i \in [d-1]$$

and therefore

$$\sum_{i=1}^{d-1} (x_{\alpha(i)} - x_{\alpha(i+1)})^2 + x_{\alpha(d)}^2 \leq N \cdot \left(\sum_{i=1}^{d-1} (x_{\alpha(i)} - x_{\alpha(i+1)}) + x_{\alpha(d)}\right) = N \cdot x_{\alpha(1)} \leq N^2.$$ 

Combining with inequality (EC.19), we get

$$\sum_{x \in \mathcal{X}} E_{M_0} [N_x(\tau)] \cdot 72\varepsilon^2 \sigma^{-2} \geq d \log \left(\frac{1}{2.4\delta}\right),$$

which implies that

$$E_{M_0}[\tau] = \sum_{x \in \mathcal{X}} E_{M_0} [N_x(\tau)] \geq \frac{d\sigma^2}{72\varepsilon^2} \log \left(\frac{1}{2.4\delta}\right).$$

\[\square\]
EC.4. Proofs in Section 6

EC.4.1. Proof of Lemma 7

Proof of Lemma 7. The proof follows the same framework as Theorem 7. We first consider points $y \in N_x$. By the condition of this lemma and inequality (15), we have

$$f(y) - f(x) \geq (1-a)^{-1} \cdot \mathbb{E}[H_x(y, \eta_y)] \geq -(1-a)^{-1}(1-a)^{-1}b.$$  

Next, we consider point $y \in X$ such that $\|y - x\|_{\infty} \leq 1$. Then, there exists two disjoint sets $S_1, S_2 \subset [d]$ such that

$$y = x + e_{S_1} - e_{S_2},$$

where $e_S := \sum_{i \in S} e_i$ is the indicator vector of $S$. Using the translation submodularity of $f(x)$, we have

$$f(y) \geq f(x + e_{S_1}) - f(x) + f(x - e_{S_2}) - f(x) \geq -2(1-a)^{-1}b.$$  

Now, let $\tilde{f}(x)$ be the convex extension of $f(x)$ defined in (12) and consider $y \in [1, N]^d$ such that $\|y - x\|_{\infty} \leq 1$. We consider the cube $C_z$ that contains both $x$ and $y$ and denote $S^{y,i}$ as the $i$-th neighboring point of $y$ in $C_z$. Recalling the expression (6), we know $f(y)$ is a convex combination of $f(S^{y,0}), \ldots, f(S^{y,d})$. Since the neighboring point $S^{y,i} \in X$ satisfies $\|S^{y,i} - x\|_{\infty} \leq 1$, we know

$$\tilde{f}(y) \geq \min_{i \in \{0\} \cup [d]} f(S^{y,i}) \geq -2(1-a)^{-1}b.$$  

Finally, we consider points $y \in [1, N]^d$. We define

$$\tilde{y} := x + \frac{y - x}{\|y - x\|_{\infty}}.$$  

Then, we know $\|\tilde{y} - x\|_{\infty} = 1$ and $\tilde{f}(\tilde{y}) \geq -2(1-a)^{-1}b$. By the convexity of $\tilde{f}(x)$,

$$\tilde{f}(y) - f(x) \geq \|y - x\|_{\infty} \left[\tilde{f}(\tilde{y}) - f(x) \right] \geq -N \cdot 2(1-a)^{-1}b = -\frac{2N}{1-a} \cdot b.$$  

□
EC.4.2. Proof of Theorem 12

Proof of Theorem 12. Let $x^*$ be a minimizer of $f(x)$. We use the induction method to prove that

$$f(x^{e,0}) - f(x^*) \leq 2^{-e} \cdot NL \quad \forall e \in \{0, 1, \ldots, E\}$$

(EC.20)

holds with probability at least $1 - e \cdot \delta/E$. Using Assumption 5, we have

$$f(x^{0,0}) - f(x^*) \leq L \cdot \|x^{0,0} - x^*\|_\infty \leq NL,$$

which means the induction assumption holds for epoch 0. Suppose the induction assumption is true for epochs $0, 1, \ldots, e - 1$. Now we consider epoch $e$. We assume the event

$$f(x^{e-1,0}) - f(x^*) \leq 2^{-e+1} \cdot NL$$

happens in the following proof, which has probability at least $1 - (e - 1)\delta/E$. We suppose epoch $e$ terminates after $T_e$ iterations and discuss by two different cases.

Case I. We first consider the case when $T_e \leq T - 1$. This event happens only if epoch $e - 1$ is terminated by the condition in Line 13, i.e.,

$$\hat{H}_{x^{e-1}, T_{e-1}}(y) > -2h_{e-1} \quad \forall y \in N_{x^{e-1}, T_{e-1}}.$$

By the definition of confidence intervals, it follows that

$$\min_{y \in N_{x^{e-1}, T_{e-1}}} \mathbb{E}[H_{x^{e-1}, T_{e-1}}(y, \eta_y)] \geq -3h_{e-1} = -3 \cdot 2^{-e-1} h_0 = -2^{-e-1} \cdot (1 - a) L$$

holds with probability at least $1 - \delta/(ET)$. Then, considering the results of Lemma 7 we know

$$f(x^{e,0}) - f(x^*) = f(x^{e-1,T_{e-1}}) - f(x^*) \leq \frac{2N}{1-a} \cdot 2^{-e-1} \cdot (1 - a) L = 2^{-e} \cdot NL$$

happens with the same probability. Combining with the induction assumption for epoch $e - 1$, the above event happens with probability at least $1 - (e - 1)\delta/E - \delta/(ET) \geq 1 - e \cdot \delta/E$ and the induction assumption holds for epoch $e$. 
Case II. Next, we consider the case when \( T_e = T \). We estimate the objective function decrease for each iteration \( t = 0, 1, \ldots, T - 1 \). By the definition of confidence intervals, it holds

\[
E[H_{x_{e-1},t}(y, \eta_y)] \leq -h_{e-1}
\]

with probability at least \( 1 - \delta/(ET) \), where \( y = x_{e-1,t+1}^{e-1} \) is the next iteration point. Recalling inequality (15), we know

\[
f(x_{e-1,t+1}^{e-1}) - f(x_{e-1,t}^{e-1}) \leq -(1 + a)^{-1} h_{e-1}
\]

happens with probability at least \( 1 - \delta/(ET) \). We assume the above event happens for all \( t = 1, 2, \ldots, T \), which has probability at least \( 1 - T \cdot \delta/(ET) = 1 - \delta/E \). Then, we have

\[
f(x_{e,0}^{e}) - f(x_{e-1,0}^{e-1}) = f(x_{e-1,T}^{e-1}) - f(x_{e-1,0}^{e-1}) = \sum_{t=1}^{T} f(x_{e-1,t}^{e-1}) - f(x_{e-1,t-1}^{e-1})
\]

\[
\leq -T \cdot (1 + a)^{-1} h_{e-1} = -2^{-e} \cdot NL
\]

holds with the same probability. Combining with the induction assumption for epoch \( e - 1 \), we know

\[
f(x_{e,0}^{e}) - f(x^{*}) \leq 2^{-e} \cdot NL
\]

happens with probability at least \( 1 - (e - 1)\delta/E - \delta/E = 1 - e \cdot \delta/E \). This means the induction assumption holds for epoch \( e \).

Combining the above two cases, we know the induction assumption is true for epoch \( e \). By the induction method, we know inequality (EC.20) holds for epoch \( E \), i.e.,

\[
f(x_{E,0}^{E}) - f(x^{*}) \leq 2^{-E} \cdot NL = 2^{-\log_2(NL/e)} \cdot NL \leq 2^{-\log_2(NL/e)} \cdot NL = \epsilon
\]

with probability at least \( 1 - E \cdot \delta/E = 1 - \delta \). Hence, Algorithm 4 returns an \((\epsilon, \delta)\)-PGS solution.

Next, we estimate the simulation cost of Algorithm 4. For each iteration in epoch \( E \), Hoeffding bound implies that simulating \( H_z(y, \eta_y) \) for

\[
\frac{2\sigma^2}{h_z^2} \log \left( \frac{2ET}{\delta} \right) = 2^{2e} \cdot \frac{288\sigma^2}{(1 - a)^2L^2} \log \left( \frac{2ET}{\delta} \right)
\]
times is sufficient to ensure that the $1 - \delta/(ET)$ confidence width is at most $T_e$. Since the simulation cost of each evaluation of all $H_x(y, \eta_y)$ is $\gamma$, the simulation cost of epoch $e$ is at most

$$
\gamma \cdot T_e \cdot 2^{2e} \cdot \frac{288\hat{s}^2}{(1-a)^2L^2} \log \left( \frac{2ET}{\delta} \right) = 2^{2e} \cdot \frac{1728(1+a)\hat{s}^2\gamma N}{(1-a)^3L^2} \log \left( \frac{2ET}{\delta} \right).
$$

Summing over $e = 0, 1, \ldots, E - 1$, we get the bound of total simulation cost as

$$
\sum_{e=0}^{E-1} 2^{2e} \cdot \frac{1728(1+a)\hat{s}^2\gamma N}{(1-a)^3L^2} \log \left( \frac{2ET}{\delta} \right) = (4^E - 1) \cdot \frac{576(1+a)\hat{s}^2\gamma N}{(1-a)^3L^2} \log \left( \frac{2ET}{\delta} \right)
\leq 4^{\left\lceil \log_2(NL/\epsilon) \right\rceil} \cdot \frac{576(1+a)\hat{s}^2\gamma N}{(1-a)^3L^2} \log \left( \frac{2ET}{\delta} \right) 
\leq \frac{4N^2L^2}{\epsilon^2} \cdot \frac{576(1+a)\hat{s}^2\gamma N}{(1-a)^3L^2} \log \left( \frac{2ET}{\delta} \right) \leq \frac{2304(1+a)\hat{s}^2\gamma N^3}{(1-a)^3\epsilon^2} \log \left( \frac{2ET}{\delta} \right).
$$

When $\delta$ is small enough, the asymptotic simulation cost is at most

$$
\frac{2304(1+a)\hat{s}^2\gamma N^3}{(1-a)^3\epsilon^2} \log \left( \frac{2ET}{\delta} \right) = \tilde{O} \left( \frac{\gamma N^3}{(1-a)^3\epsilon^2} \log \left( \frac{1}{\delta} \right) \right).
$$

□

**EC.4.3. Proof of Theorem 13**

**Proof of Theorem 13.** If the algorithm terminates before the $T$-th iteration, then the condition at Line 11 is satisfied for the last iteration point, which we denote as $x^t$. Let

$$
y^t := \arg\min_{y \in \mathcal{N}_{x^t}} f(y).
$$

Then, by the definition of confidence intervals, it holds

$$
\mathbb{E}[H_{x^{t-1}}(y^t, \eta_{y^t})] \geq -3h
$$

with probability at least $1 - \delta/(2T) \geq 1 - \delta$. By inequality (15), we know

$$
\min_{y \in \mathcal{N}_{x^t}} f(y) - f(x^t) = f(y^t) - f(x^t) \geq -\frac{3h}{1-a} = -\frac{c}{4}
$$

holds with the same probability. We assume the event happens in the following proof. For any point $y \in \mathcal{X}$ such that $\|y - x^t\|_\infty \leq 1$, there exists two disjoint sets $S_1, S_2 \subset [d]$ such that

$$
y = x^t + e_{S_1} - e_{S_2},
$$
where \( e_S := \sum_{i \in S} e_i \) is the indicator vector of \( S \). Then, using the \( L^3 \)-convexity of \( f(x) \), we know

\[
f(y) - f(x^t) \geq f(x^t + e_{S_1}) - f(x^t) + f(x^t - e_{S_2}) - f(x^t) \geq -\frac{c}{2}.
\]

Let \( \tilde{f}(x) \) be the convex extension of \( f(x) \) defined in (12). Recalling expression (6), we know

\[
\tilde{f}(y) - f(x^t) \geq -\frac{c}{2} \quad \forall y \in [1, N]^d \quad \text{s.t.} \quad \|y - x^t\|_\infty \leq 1. 
\]

(EC.21)

We assume that \( x^t \) is not the minimizer of \( f(x) \), which we denote as \( x^* \). Since the indifference zone parameter is \( c \), we know

\[
f(y) - f(x^*) \geq -c \quad \forall y \in \mathcal{X}\backslash\{x^*\}. 
\]

(EC.22)

Similarly, using expression (6), we get

\[
\tilde{f}(y) - f(x^*) \geq -c \quad \forall y \in [1, N]^d \quad \text{s.t.} \quad \|y - x^*\|_\infty \leq 1. 
\]

If \( \|x^t - x^*\|_\infty \leq 1 \), then there exists a point \( x^* \) such that \( \|x^* - x^t\|_\infty \leq 1 \) and

\[
f(x^*) - f(x^t) \leq -c,
\]

which contradicts with inequality (EC.21). Otherwise if \( \|x^t - x^*\|_\infty \geq 2 \), we define

\[
x^{t,1} := x^t + \frac{x^* - x^t}{\|x^t - x^*\|_\infty}, \quad x^{t,2} := x^* + \frac{x^t - x^*}{\|x^* - x^t\|_\infty}
\]

Then, it holds

\[
\|x^t - x^{t,1}\|_\infty = 1, \quad \|x^* - x^{t,2}\|_\infty = 1
\]

and \( x^{t,1}, x^{t,2} \) are closer to \( x^t, x^* \), respectively. By inequalities (EC.21) and (EC.22), we get

\[
\tilde{f}(x^{t,1}) - f(x^t) \geq -\frac{c}{2}, \quad \tilde{f}(x^*) - f(x^{t,2}) \leq -c.
\]

However, the convexity of \( \tilde{f}(x) \) on the segment \( x^t x^* \) implies that

\[
-\frac{c}{2} \leq \tilde{f}(x^{t,1}) - f(x^t) \leq \tilde{f}(x^*) - f(x^{t,2}) \leq -c.
\]
which is a contradiction. Hence, we know $x^t = x^*$ is the minimizer of $f(x)$. This event happens with probability at least $1 - \delta$ and therefore $x^t$ is a $(c, \delta)$-PCS-IZ solution.

Otherwise, we assume the algorithm terminates after $T$ iterations. We use the induction method to prove that

$$f(x^t) - f(x^0) \leq -t \cdot \frac{(1 - a)c}{12(1 + a)}$$

happens with probability at least $1 - t \cdot \delta/(2T)$. For the initial point $x^0$, this claim holds trivially. Suppose the induction assumption is true for $x^0, x^1, \ldots, x^{t-1}$. For the $(t-1)$-th iteration, by the definition of confidence intervals, it holds

$$\mathbb{E}[H_{x^{t-1}}(x^t, \eta_{x^t})] \leq -h$$

with probability at least $1 - \delta/(2T)$. Using inequality [15], we know

$$f(x^t) - f(x^{t-1}) \leq -\frac{h}{1 + a} = -\frac{(1 - a)c}{12(1 + a)}$$

holds with the same probability. Using the induction assumption for $x^{t-1}$, we have

$$f(x^t) - f(x^0) \leq -(t - 1) \cdot \frac{(1 - a)c}{12(1 + a)} - \frac{(1 - a)c}{12(1 + a)} = -t \cdot \frac{(1 - a)c}{12(1 + a)}$$

holds with probability at least $1 - (t - 1)\delta/(2T) - \delta/(2T) = 1 - t \cdot \delta/(2T)$. Hence, the induction assumption holds for $x^t$ and, by the induction method, holds for all iterations. Since the algorithm terminates after $T$ iterations, the last point $x^T$ satisfies

$$f(x^T) - f(x^0) \leq -T \cdot \frac{(1 - a)c}{12(1 + a)} = -cN$$

with probability at least $1 - T \cdot \delta/(2T) = 1 - \delta/2$. Recalling the initial point $x^0$ is a $(cN, \delta/2)$-PGS solution, we know $x^T$ is the optimal point with probability at least $1 - \delta$ and therefore is a $(c, \delta)$-PCS-IZ solution.

Finally, we estimate the simulation cost of Algorithm\[5\] By Theorem\[12\] the simulation cost for generating the initial point is

$$\mathcal{O} \left[ \frac{\gamma N}{(1 - a)^3c^2} \log \left( \frac{1}{\delta} \right) \right].$$
For each iteration, Hoeffding bound implies that simulating
\[
\frac{2\tilde{\sigma}^2}{h^2 \log\left(\frac{4T}{\delta}\right)} = \frac{288\tilde{\sigma}^2}{(1-a)^2 c^2 \log\left(\frac{4T}{\delta}\right)}
\]
times is enough for the \(1 - \delta/(2T)\) confidence width to be smaller than \(h\). Hence, the total simulation for iterations is at most
\[
T \cdot \gamma \cdot \frac{288\tilde{\sigma}^2}{(1-a)^2 c^2 \log\left(\frac{4T}{\delta}\right)} = \frac{1152\gamma\tilde{\sigma}^2 (1+a)N}{(1-a)^3 c^2 \log\left(\frac{4T}{\delta}\right)} = O\left[\frac{\gamma N}{(1-a)^3 c^2 \log\left(\frac{1}{\delta}\right)}\right].
\]
Combining the simulation costs for initialization and iterations, we know the asymptotic simulation cost of Algorithm 5 is at most
\[
\bar{O}\left[\frac{\gamma N}{(1-a)^3 c^2 \log\left(\frac{1}{\delta}\right)}\right].
\]