Black Box Submodular Maximization: Discrete and Continuous Settings

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Abstract

In this paper, we consider the problem of black box continuous submodular maximization where we only have access to the function values and no information about the derivatives is provided. For a monotone and continuous DR-submodular function, and subject to a bounded convex body constraint, we propose Black-box Continuous Greedy, a derivative-free algorithm that provably achieves the tight $[(1-1/e)OPT-\epsilon]$ approximation guarantee with $O(d/\epsilon^3)$ function evaluations. We then extend our result to the stochastic setting where function values are subject to stochastic zero-mean noise. It is through this stochastic generalization that we revisit the discrete submodular maximization problem and use the multi-linear extension as a bridge between discrete and continuous settings. Finally, we extensively evaluate the performance of our algorithm on continuous and discrete submodular objective functions using both synthetic and real data.

1 Introduction

Black-box optimization, also known as zeroth-order or derivative-free optimization[2], has been extensively studied in the literature [Conn et al., 2009, Bergstra et al., 2011, Rios and Sahinidis, 2013, Shahriari et al., 2016]. In this setting, we assume that the objective function is unknown and we can only obtain zeroth-order information such as (stochastic) function evaluations.

Fueled by a growing number of machine learning applications, black-box optimization methods are usually considered in scenarios where gradients (*i.e.*, first-order information) are 1) difficult or slow to compute, *e.g.*, graphical model inference [Wainwright et al., 2008], structure predictions [Taskar et al., 2005, Sokolov et al., 2016], or 2) inaccessible, *e.g.*, hyper-parameter turning for natural language processing or image classifications Snoek et al. [2012], Thornton et al. [2013], black-box attacks for finding adversarial examples Chen et al. [2017c], Ilyas et al. [2018]. Even though heuristics such as random or grid search, with undesirable dependencies on the dimension, are still used in some applications (*e.g.*, parameter tuning for deep networks), there has been a growing number of rigorous methods to address the convergence rate of black-box optimization in convex and non-convex settings [Wang et al., 2017, Balasubramanian and Ghadimi, 2018, Sahu et al., 2018].

The focus of this paper is the *constrained* continuous DR-submodular maximization over a bounded convex body. We aim to design an algorithm that uses only zeroth-order information while avoiding expensive projection operations. Note that one way the optimization methods can deal with constraints is to apply the projection oracle once the proposed iterates land outside the feasibility region. However, computing the projection in many constrained settings is computationally prohibitive (*e.g.*, projection over bounded trace norm matrices, flow polytope, matroid polytope, rotation matrices). In such scenarios, projection-free algorithms, *a.k.a.*, Frank-Wolfe [Frank and Wolfe, 1956], replace

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[2] We note that black-box optimization (BBO) and derivative-free optimization (DFO) are not identical terms. Audet and Hare [2017] defined DFO as "the mathematical study of optimization algorithms that do not use derivatives" and BBO as "the study of design and analysis of algorithms that assume the objective and/or constraint functions are given by blackboxes". However, as the differences are nuanced in most scenarios, this paper uses them interchangeably.

Proceedings of the 23rd International Conference on Artificial Intelligence and Statistics (AISTATS) 2020, Palermo, Italy. PMLR: Volume 108.

Table 1: Number of function queries in different settings, where D_1 is the diameter of $\mathcal{K}$.

Function	Additional Assumptions	Function Queries
continuous DR-submodular	monotone, G-Lipschitz, L-smooth	$\mathcal{O}(\max\{G, LD_1\}^3 \cdot \frac{d}{\epsilon^3})$ [Theorem 1]
stoch. continuous DR-submodular	monotone, G-Lipschitz, L-smooth	$\mathcal{O}(\max\{G, LD_1\}^3 \cdot \frac{d^3}{\epsilon^5})$ [Theorem 2]
discrete submodular	monotone	$\mathcal{O}(\frac{d^5}{\epsilon^5})$ [Theorem 3]

the projection with a linear program. Indeed, our proposed algorithm combines efficiently the zeroth-order information with solving a series of linear programs to ensure convergence to a near-optimal solution.

Continuous DR-submodular functions are an important subset of non-convex functions that can be minimized exactly Bach [2016], Staib and Jegelka [2017] and maximized approximately Bian et al. [2017a,b], Hassani et al. [2017], Mokhtari et al. [2018a], Hassani et al. [2019], Zhang et al. [2019b] This class of functions generalize the notion of diminishing returns, usually defined over discrete set functions, to the continuous domains. They have found numerous applications in machine learning including MAP inference in determinantal point processes (DPPs) Kulesza et al. [2012], experimental design Chen et al. [2018c], resource allocation Eghbali and Fazel [2016], mean-field inference in probabilistic models Bian et al. [2018], among many others.

Motivation: Computing the gradient of a continuous DR-submodular function has been shown to be computationally prohibitive (or even intractable) in many applications. For example, the objective function of influence maximization is defined via specific stochastic processes [Kempe et al., 2003, Rodriguez and Schölkopf, 2012] and computing/estimating the gradient of the mutliliear extension would require a relatively high computational complexity. In the problem of D-optimal experimental design , the gradient of the objective function involves inversion of a potentially large matrix [Chen et al., 2018c]. Moreover, when one attacks a submodular recommender model, only black-box information is available and the service provider is unlikely to provide additional first-order information (this is known as the black-box adversarial attack model) [Lei et al., 2019].

There has been very recent progress on developing zeroth-order methods for constrained optimization problems in convex and non-convex settings Ghadimi and Lan [2013], Sahu et al. [2018]. Such methods typically assume the objective function is defined on the whole $\mathbb{R}^d$ so that they can sample points from a proper distribution defined on $\mathbb{R}^d$. For DR-submodular functions, this assumption might be unrealistic, since many DR-submodular functions might be only defined on a subset of $\mathbb{R}^d$, *e.g.*, the multi-linear extension Vondrák [2008], a canonical example of DR-submodular functions, is only defined on a unit cube. Moreover, they can only guarantee to reach a first-order stationary point. However, Hassani et al. [2017] showed that for a monotone DR-submodular function, the stationary points can only guarantee $1/2$ approximation to the optimum. Therefore, if a state-of-the-art zeroth-order non-convex algorithm is used for maximizing a monotone DR-submodular function, it is likely to terminate at a suboptimal stationary point whose approximation ratio is only $1/2$.

Our contributions: In this paper, we propose a derivative-free and projection-free algorithm Black-box Continuous Greedy (BCG), that maximizes a monotone continuous DR-submodular function over a bounded convex body $\mathcal{K} \subseteq \mathbb{R}^d$. We consider three scenarios:

(1) In the deterministic setting, where function evaluations can be obtained exactly, BCG achieves the tight $[(1-1/e)OPT-\epsilon]$ approximation guarantee with $\mathcal{O}(d/\epsilon^3)$ function evaluations.

(2) In the stochastic setting, where function evaluations are noisy, BCG achieves the tight $[(1-1/e)OPT-\epsilon]$ approximation guarantee with $\mathcal{O}(d^3/\epsilon^5)$ function evaluations.

(3) In the discrete setting, Discrete Black-box Greedy (DBG) achieves the tight $[(1-1/e)OPT-\epsilon]$ approximation guarantee with $\mathcal{O}(d^5/\epsilon^5)$ function evaluations.

All the theoretical results are summarized in Table 1.

We would like to note that in discrete setting, due to the conservative upper bounds for the Lipschitz and smooth parameters of general multilinear extensions, and the variance of the gradient estimators subject to noisy function evaluations, the required number of function queries in theory is larger than the best known result, $\mathcal{O}(d^{5/2}/\epsilon^3)$ in Mokhtari et al. [2018a,b]. However, our experiments show that empirically, our proposed algorithm often requires significantly fewer function evaluations and less running time, while achieving a practically similar utility.

Novelty of our work: All the previous results in constrained DR-submodular maximization assume access to (stochastic) gradients. In this work, we address a harder problem, *i.e.*, we provide the first rigorous analysis when only (stochastic) function values can be obtained. More specifically, with the smoothing trick [Flaxman et al., 2005], one can construct an unbiased gradient estimator via function queries. However, this estimator has a large $\mathcal{O}(d^2/\delta^2)$ variance which may cause FW-type methods to diverge. To overcome this issue, we build on the momentum method proposed by Mokhtari et al. [2018a] in which they assumed access to the *first-order* information.

Given a point x, the smoothed version of F at x is defined as $\mathbb{E}_{v\sim B^d}[F(x+\delta v)]$. If x is close to the boundary of the domain $\mathcal{D}$, $(x+\delta v)$ may fall outside of $\mathcal{D}$, leaving the smoothed function undefined for many instances of DR-submodular functions (*e.g.*, the multilinear extension is only defined over the unit cube). Thus the vanilla smoothing trick will not work. To this end, we transform the domain $\mathcal{D}$ and constraint set $\mathcal{K}$ in a proper way and run our zeroth-order method on the transformed constraint set $\mathcal{K}'$. Importantly, we retrieve the same convergence rate of $\mathcal{O}(T^{-1/3})$ as in Mokhtari et al. [2018a] with a minimum number of function queries in different settings (continuous, stochastic continuous, discrete).

We further note that by using more recent variance reduction techniques [Zhang et al., 2019b], one might be able to reduce the required number of function evaluations.

1.1 Further Related Work

Submodular functions Nemhauser et al. [1978], that capture the intuitive notion of diminishing returns, have become increasingly important in various machine learning applications. Examples include graph cuts in computer vision Jegelka and Bilmes [2011a,b], data summarization Lin and Bilmes [2011b,a], Tschiatschek et al. [2014], Chen et al. [2018a, 2017b], influence maximization Kempe et al. [2003], Rodriguez and Schölkopf [2012], Zhang et al. [2016], feature compression Bateni et al. [2019], network inference Chen et al. [2017a], active and semi-supervised learning Guillory and Bilmes [2010], Golovin and Krause [2011], Wei et al. [2015], crowd teaching Singla et al. [2014], dictionary learning Das and Kempe [2011], fMRI parcellation Salehi et al. [2017], compressed sensing and structured sparsity Bach [2010], Bach et al. [2012], fairness in machine learning Balkanski and Singer [2015], Celis et al. [2016], and learning causal structures Steudel et al. [2010], Zhou and Spanos [2016], to name a few. Continuous DR-submodular functions naturally extend the notion of diminishing returns to the continuous domains Bian et al. [2017b]. Monotone continuous DR-submodular functions can be (approximately) maximized over convex bodies using first-order methods Bian et al. [2017b], Hassani et al. [2017], Mokhtari et al. [2018a]. Bandit maximization of monotone continuous DR-submodular functions Zhang et al. [2019a] is a closely related setting to ours. However, to the best of our knowledge, none of the existing work has developed a zeroth-order algorithm for maximizing a monotone continuous DR-submodular function. For a detailed review of DFO and BBO, interested readers refer to book [Audet and Hare, 2017].

2 Preliminaries

Submodular Functions We say a set function $f : 2^\Omega \to \mathbb{R}$ is submodular, if it satisfies the diminishing returns property: for any $A \subseteq B \subseteq \Omega$ and $x \in \Omega \setminus B$, we have

$$f(A \cup \{x\}) - f(A) \geq f(B \cup \{x\}) - f(B). \quad (1)$$

In words, the marginal gain of adding an element x to a subset A is no less than that of adding x to its superset B.

For the continuous analogue, consider a function $F : \mathcal{X} \to \mathbb{R}_+$, where $\mathcal{X} = \Pi_{i=1}^n \mathcal{X}_i$, and each $\mathcal{X}_i$ is a compact subset of $\mathbb{R}_+$. We define F to be continuous submodular if F is continuous and for all $x, y \in \mathcal{X}$, we have

$$F(x) + F(y) \geq F(x \vee y) + F(x \wedge y), \quad (2)$$

where $\vee$ and $\wedge$ are the component-wise maximizing and minimizing operators, respectively.

The continuous function F is called DR-submodular Bian et al. [2017b] if F is differentiable and $\forall\, x \leq y$: $\nabla F(x) \geq \nabla F(y)$. An important implication of DR-submodularity is that the function F is concave in any non-negative directions, *i.e.*, for $x \leq y$, we have

$$F(y) \leq F(x) + \langle \nabla F(x), y - x \rangle. \quad (3)$$

The function F is called monotone if for $x \leq y$, we have $F(x) \leq F(y)$.

Smoothing Trick For a function F defined on $\mathbb{R}^d$, its δ-smoothed version is given as

$$\tilde{F}_\delta(x) \triangleq \mathbb{E}_{v\sim B^d}[F(x + \delta v)], \quad (4)$$

where v is chosen uniformly at random from the d-dimensional unit ball B^d. In words, the function $\tilde{F}_\delta$ at any point x is obtained by "averaging" F over a ball of radius δ around x. In the sequel, we omit the subscript δ for the sake of simplicity and use $\tilde{F}$ instead of $\tilde{F}_\delta$.

Lemma 1 below shows that under the Lipschitz assumption for F, the smoothed version $\tilde{F}$ is a good approximation of F, and also inherits the key structural properties of F (such as monotonicity and submodularity). Thus one can (approximately) optimize F via optimizing $\tilde{F}$.

Lemma 1 (Proof in Appendix A). *If F is monotone continuous DR-submodular and G-Lipschitz continuous on $\mathbb{R}^d$, then so is $\tilde{F}$ and*

$$|\tilde{F}(x) - F(x)| \leq \delta G. \tag{5}$$

An important property of $\tilde{F}$ is that one can obtain an unbiased estimation for its gradient $\nabla \tilde{F}$ by a single query of F. This property plays a key role in our proposed derivative-free algorithms.

Lemma 2 (Lemma 6.5 in [Hazan, 2016]). *Given a function F on $\mathbb{R}^d$, if we choose u uniformly at random from the $(d-1)$-dimensional unit sphere S^{d-1}, then we have*

$$\nabla \tilde{F}(x) = \mathbb{E}_{u \sim S^{d-1}} \left[\frac{d}{\delta} F(x + \delta u) u \right]. \tag{6}$$

3 DR-Submodular Maximization

In this paper, we mainly focus on the constrained optimization problem:

$$\max_{x \in \mathcal{K}} F(x), \tag{7}$$

where F is a monotone continuous DR-submodular function on $\mathbb{R}^d$, and the constraint set $\mathcal{K} \subseteq \mathcal{X} \subseteq \mathbb{R}^d$ is convex and compact.

For *first-order* monotone DR-submodular maximization, one can use Continuous Greedy Calinescu et al. [2011], Bian et al. [2017b], a variant of Frank-Wolfe Algorithm [Frank and Wolfe, 1956, Jaggi, 2013, Lacoste-Julien and Jaggi, 2015], to achieve the $[(1-1/e)OPT - \epsilon]$ approximation guarantee. At iteration t, the FW variant first maximizes the linearization of the objective function F:

$$v_t = \arg\max_{v \in \mathcal{K}} \langle v, \nabla F(x_t) \rangle. \tag{8}$$

Then the current point x_t moves in the direction of v_t with a step size $\gamma_t \in (0, 1]$:

$$x_{t+1} = x_t + \gamma_t v_t. \tag{9}$$

Hence, by solving linear optimization problems, the iterates are updated without resorting to the projection oracle.

Here we introduce our main algorithm Black-box Continuous Greedy which assumes access only to function values (*i.e.*, zeroth-order information). This algorithm is partially based on the idea of Continuous Greedy. The basic idea is to utilize the function evaluations of F at carefully selected points to obtain unbiased estimations of the gradient of the smoothed version, $\nabla \tilde{F}$. By extending Continuous Greedy to the derivative-free setting and using recently proposed variance reduction techniques, we can then optimize $\tilde{F}$ near-optimally. Finally, by Lemma 1 we show that the obtained optimizer also provides a good solution for F.

Recall that continuous DR-submodular functions are defined on a box $\mathcal{X} = \Pi_{i=1}^n \mathcal{X}_i$. To simplify the exposition, we can assume, without loss of generality, that the objective function F is defined on $\mathcal{D} \triangleq \prod_{i=1}^d [0, a_i]$ Bian et al. [2017a]. Moreover, we note that since $\tilde{F} = \mathbb{E}_{v \sim B^d}[F(x + \delta v)]$, for x close to $\partial \mathcal{D}$ (the boundary of $\mathcal{D}$), the point $x + \delta v$ may fall outside of $\mathcal{D}$, leaving the function $\tilde{F}$ undefined.

To circumvent this issue, we shrink the domain $\mathcal{D}$ by δ. Precisely, the shrunk domain is defined as

$$\mathcal{D}'_\delta = \{x \in \mathcal{D} | d(x, \partial \mathcal{D}) \geq \delta\}. \tag{10}$$

Since we assume $\mathcal{D} = \prod_{i=1}^d [0, a_i]$, the shrunk domain is $\mathcal{D}'_\delta = \prod_{i=1}^d [\delta, a_i - \delta]$. Then for all $x \in \mathcal{D}'_\delta$, we have $x + \delta v \in \mathcal{D}$. So $\tilde{F}$ is well-defined on $\mathcal{D}'_\delta$. By Lemma 1, the optimum of $\tilde{F}$ on the shrunk domain $\mathcal{D}'_\delta$ will be close to that on the original domain $\mathcal{D}$, if δ is small enough. Therefore, we can first optimize $\tilde{F}$ on $\mathcal{D}'_\delta$, then approximately optimize $\tilde{F}$ (and thus F) on $\mathcal{D}$. For simplicity of analysis, we also translate the shrunk domain $\mathcal{D}'_\delta$ by $-\delta$, and denote it as $\mathcal{D}_\delta = \prod_{i=1}^d [0, a_i - 2\delta]$.

Besides the domain $\mathcal{D}$, we also need to consider the transformation on constraint set $\mathcal{K}$. Intuitively, if there is no translation, we should consider the intersection of $\mathcal{K}$ and the shrunk domain $\mathcal{D}'_\delta$. But since we translate $\mathcal{D}'_\delta$ by $-\delta$, the same transformation should be performed on $\mathcal{K}$. Thus, we define the transformed constraint set as the translated intersection (by $-\delta$) of $\mathcal{D}'_\delta$ and $\mathcal{K}$:

$$\mathcal{K}' \triangleq (\mathcal{D}'_\delta \cap \mathcal{K}) - \delta \mathbf{1} = \mathcal{D}_\delta \cap (\mathcal{K} - \delta \mathbf{1}). \tag{11}$$

It is well known that the FW Algorithm is sensitive to the accuracy of gradient, and may have arbitrarily poor performance with stochastic gradients Hazan and Luo [2016], Mokhtari et al. [2018b]. Thus we incorporate two methods of variance reduction into our proposed algorithm Black-box Continuous Greedy which correspond to Step 7 and Step 8 in Algorithm 1, respectively. First, instead of the one-point gradient estimation in Lemma 2, we adopt the two-point estimator of $\nabla \tilde{F}(x)$ [Agarwal et al., 2010, Shamir, 2017]:

$$\frac{d}{2\delta}(F(x + \delta u) - F(x - \delta u))u, \tag{12}$$

where u is chosen uniformly at random from the unit sphere S^{d-1}.We note that (12) is an unbiased gradient estimator with less variance w.r.t. the one-point estimator. We also average over a mini-batch of B_t

Algorithm 1 Black-box Continuous Greedy

1: **Input:** constraint set $\mathcal{K}$, iteration number T, radius δ, step size ρ_t, batch size B_t
2: **Output:** $x_{T+1} + \delta \mathbf{1}$
3: $x_1 \leftarrow \mathbf{0}$, $\bar{g}_0 \leftarrow \mathbf{0}$
4: **for** $t = 1$ **to** T **do**
5: Sample $u_{t,1}, \ldots, u_{t,B_t}$ i.i.d. from S^{d-1}
6: For $i = 1$ to B_t, let $y_{t,i}^+ \leftarrow \delta \mathbf{1} + x_t + \delta u_{t,i}$, $y_{t,i}^- \leftarrow \delta \mathbf{1} + x_t - \delta u_{t,i}$ and evaluate $F(y_{t,i}^+), F(y_{t,i}^-)$
7: $g_t \leftarrow \frac{1}{B_t} \sum_{i=1}^{B_t} \frac{d}{2\delta} [F(y_{t,i}^+) - F(y_{t,i}^-)] u_{t,i}$
8: $\bar{g}_t \leftarrow (1 - \rho_t) \bar{g}_{t-1} + \rho_t g_t$
9: $v_t \leftarrow \arg\max_{v \in \mathcal{K}'} \langle v, \bar{g}_t \rangle$
10: $x_{t+1} \leftarrow x_t + \frac{v_t}{T}$
11: **end for**
12: Output $x_{T+1} + \delta \mathbf{1}$

independently sampled two-point estimators for further variance reduction. The second variance-reduction technique is the momentum method used in [Mokhtari et al., 2018a] to estimate the gradient by a vector $\bar{g}_t$ which is updated at each iteration as follows:

$$\bar{g}_t = (1 - \rho_t) \bar{g}_{t-1} + \rho_t g_t. \tag{13}$$

Here ρ_t is a given step size, $\bar{g}_0$ is initialized as an all zero vector $\mathbf{0}$, and g_t is an unbiased estimate of the gradient at iterate x_t. As $\bar{g}_t$ is a weighted average of previous gradient approximation $\bar{g}_{t-1}$ and the newly updated stochastic gradient g_t, it has a lower variance compared with g_t. Although $\bar{g}_t$ is not an unbiased estimation of the true gradient, the error of it will approach zero as time proceeds. The detailed description of Black-box Continuous Greedy is provided in Algorithm 1.

Theorem 1 (Proof in Appendix B)**.** *For a monotone continuous DR-submodular function F, which is also G-Lipschitz continuous and L-smooth on a convex and compact constraint set $\mathcal{K}$, if we set $\rho_t = 2/(t+3)^{2/3}$ in Algorithm 1, then we have*

$$\begin{aligned}&(1 - 1/e) F(x^*) - \mathbb{E}[F(x_{T+1} + \delta \mathbf{1})] \\ &\leq \frac{3 D_1 Q^{1/2}}{T^{1/3}} + \frac{L D_1^2}{2T} + \delta G (1 + (\sqrt{d} + 1)(1 - 1/e)).\end{aligned}$$

where $Q = \max\{4^{2/3} G^2, 4cdG^2/B_t + 6L^2 D_1^2\}$, c is a constant, $D_1 = \mathrm{diam}(\mathcal{K}')$, and x^* is the global maximizer of F on $\mathcal{K}$.

Remark 1. *By setting $T = \mathcal{O}(1/\epsilon^3)$, $B_t = d$, and $\delta = \epsilon/\sqrt{d}$, the error term (RHS) is guaranteed to be at most $\mathcal{O}(\epsilon)$. Also, the total number of function evaluations is at most $\mathcal{O}(d/\epsilon^3)$.*

We can also extend Algorithm 1 to the stochastic case in which we obtain information about F only through its noisy function evaluations $\hat{F}(x) = F(x) + \xi$, where ξ is stochastic zero-mean noise. In particular, in Step 6 of Algorithm 1, we obtain independent stochastic function evaluations $\hat{F}(y_{t,i}^+)$ and $\hat{F}(y_{t,i}^-)$, instead of the exact function values $F(y_{t,i}^+)$ and $F(y_{t,i}^-)$. For unbiased function evaluation oracles with uniformly bounded variance, we have the following theorem.

Theorem 2 (Proof in Appendix C)**.** *Under the condition of Theorem 1, if we further assume that for all x, $\mathbb{E}[\hat{F}(x)] = F(x)$ and $\mathbb{E}[|\hat{F}(x) - F(x)|^2] \leq \sigma_0^2$, then we have*

$$\begin{aligned}&(1 - 1/e) F(x^*) - \mathbb{E}[F(x_{T+1} + \delta \mathbf{1})] \\ &\leq \frac{3 D_1 Q^{1/2}}{T^{1/3}} + \frac{L D_1^2}{2T} + \delta G (1 + (\sqrt{d} + 1)(1 - 1/e)),\end{aligned}$$

where $D_1 = \mathrm{diam}(\mathcal{K}')$, $Q = \max\{4^{2/3} G^2, 6L^2 D_1^2 + (4cdG^2 + 2d^2\sigma_0^2/\delta^2)/B_t\}$, c is a constant, and x^* is the global maximizer of F on $\mathcal{K}$.

Remark 2. *By setting $T = \mathcal{O}(1/\epsilon^3)$, $B_t = d^3/\epsilon^2$, and $\delta = \epsilon/\sqrt{d}$, the error term (RHS) is at most $\mathcal{O}(\epsilon)$. The total number of evaluations is at most $\mathcal{O}(d^3/\epsilon^5)$.*

4 Discrete Submodular Maximization

In this section, we describe how Black-box Continuous Greedy can be used to solve a discrete submodular maximization problem with a general matroid constraint, *i.e.*, $\max_{S \in \mathcal{I}} f(S)$, where f is a monotone submodular set function and $\mathcal{I}$ is a matroid.

For any monotone submodular set function $f : 2^\Omega \to \mathbb{R}_{\geq 0}$, its multilinear extension $F : [0,1]^d \to \mathbb{R}_{\geq 0}$, defined as

$$F(x) = \sum_{S \subseteq \Omega} f(S) \prod_{i \in S} x_i \prod_{j \notin S} (1 - x_j), \tag{14}$$

is monotone and DR-submodular [Calinescu et al., 2011]. Here, $d = |\Omega|$ is the size of the ground set Ω. Equivalently, we have $F(x) = \mathbb{E}_{S \sim x}[f(S)]$, where $S \sim x$ means that the each element $i \in \Omega$ is included in S with probability x_i independently.

It can be shown that in lieu of solving the discrete optimization problem one can solve the continuous optimization problem $\max_{x \in \mathcal{K}} F(x)$, where $\mathcal{K} = \mathrm{conv}\{1_I : I \in \mathcal{I}\}$ is the matroid polytope [Calinescu et al., 2011]. This equivalence is obtained by showing that (i) the optimal values of the two problems are the same, and (ii) for any fractional vector $x \in \mathcal{K}$ we can deploy efficient, lossless rounding procedures that produce a set $S \in \mathcal{I}$ such that $\mathbb{E}[f(S)] \geq F(x)$ (*e.g.*, pipage rounding [Ageev and Sviridenko, 2004, Calinescu et al., 2011] and contention resolution [Chekuri et al., 2014]). So we can view $\tilde{F}$ as the underlying function that we intend to optimize, and invoke Black-box Continuous Greedy. As

Algorithm 2 Discrete Black-box Greedy

Input: matroid constraint $\mathcal{I}$, transformed constraint set $\mathcal{K}' = \mathcal{D}_\delta \cap (\mathcal{K} - \delta\mathbf{1})$ where $\mathcal{K} = \text{conv}\{1_I : I \in \mathcal{I}\}$, number of iterations T, radius δ, step size ρ_t, batch size B_t, sample size $S_{t,i}$
Output: X_{T+1}
$x_1 \leftarrow \mathbf{0}$, $\bar{g}_0 \leftarrow \mathbf{0}$,
for $t = 1$ **to** T **do**
  Sample $u_{t,1}, \dots, u_{t,B_t}$ i.i.d. from S^{d-1}
  For $i = 1$ to B_t, let $y^+_{t,i} \leftarrow \delta\mathbf{1} + x_t + \delta u_{t,i}, y^-_{t,i} \leftarrow \delta\mathbf{1} + x_t - \delta u_{t,i}$, independently sample subsets $Y^+_{t,i}$ and $Y^-_{t,i}$ for $S_{t,i}$ times according to $y^+_{t,i}, y^-_{t,i}$, get sampled subsets $Y^+_{t,i,j}, Y^-_{t,i,j}, \forall j \in [S_{t,i}]$, evaluate the function values $f(Y^+_{t,i,j}), f(Y^-_{t,i,j}), \forall j \in [S_{t,i}]$, and calculate the averages $\bar{f}^+_{t,i} \leftarrow \frac{\sum_{j=1}^{S_{t,i}} f(Y^+_{t,i,j})}{S_{t,i}}, \bar{f}^-_{t,i} \leftarrow \frac{\sum_{j=1}^{S_{t,i}} f(Y^-_{t,i,j})}{S_{t,i}}$
  $g_t \leftarrow \frac{1}{B_t} \sum_{i=1}^{B_t} \frac{d}{2\delta} (\bar{f}^+_{t,i} - \bar{f}^-_{t,i}) u_{t,i}$
  $\bar{g}_t \leftarrow (1 - \rho_t)\bar{g}_{t-1} + \rho_t g_t$
  $v_t \leftarrow \arg\max_{v \in \mathcal{K}'} \langle v, \bar{g}_t \rangle$
  $x_{t+1} \leftarrow x_t + \frac{v_t}{T}$
end for
Output $X_{T+1} = \text{round}(x_{T+1} + \delta\mathbf{1})$

a result, we want that F is G-Lipschitz and L-smooth as in Theorem 1. The following lemma shows these properties are satisfied automatically if f is bounded.

Lemma 3. *For a submodular set function f defined on Ω with $\sup_{X \subseteq \Omega} |f(X)| \leq M$, its multilinear extension F is $2M\sqrt{d}$-Lipschitz and $4M\sqrt{d(d-1)}$-smooth.*

We note that the bounds for Lipschitz and smoothness parameters actually depend on the norms that we consider. However, different norms are equivalent up to a factor that may depend on the dimension. If we consider another norm, some dimension factors may be absorbed into the norm. Therefore, we only study the Euclidean norm in Lemma 3.

We further note that computing the exact value of F is difficult as it requires evaluating f over all the subsets $S \in \Omega$. However, one can construct an unbiased estimate for the value $F(x)$ by simply sampling a random set $S \sim x$ and returning $f(S)$ as the estimate. We present our algorithm in detail in Algorithm 2, where we have $\mathcal{D} = [0,1]^d$, since F is defined on $[0,1]^d$, and thus $\mathcal{D}_\delta = [0, 1 - 2\delta]^d$. We state the theoretical result formally in Theorem 3.

Theorem 3 (Proof in Appendix E)**.** *For a monotone submodular set function f with $\sup_{X \subseteq \Omega} |f(X)| \leq M$, if we set $\rho_t = 2/(t+3)^{2/3}, S_{t,i} = l$ in Algorithm 2, then we have*

$$\begin{aligned}(1 - 1/e)f(X^*) - \mathbb{E}[f(X_{T+1})] \\ \leq \frac{3D_1 Q^{1/2}}{T^{1/3}} + \frac{2M\sqrt{d(d-1)}D_1^2}{T} \\ + 2M\delta\sqrt{d}(1 + (\sqrt{d} + 1)(1 - 1/e)).\end{aligned}$$

where $D_1 = \text{diam}(\mathcal{K}')$, $Q = \max\{\frac{2d^2M^2(\frac{1}{l\delta^2} + 8c)}{B_t} + 96d(d-1)M^2D_1^2, 4^{5/3}dM^2\}, c$ is a constant, X^* is the global maximizer of f under matroid constraint $\mathcal{I}$.

Remark 3. *By setting $T = \mathcal{O}(d^3/\epsilon^3)$, $B_t = 1, l = d^2/\epsilon^2$, and $\delta = \epsilon/d$, the error term (RHS) is at most $\mathcal{O}(\epsilon)$. The total number of evaluations is at most $\mathcal{O}(d^5/\epsilon^5)$.*

We note that in Algorithm 2, $\bar{f}^+_{t,i}$ is the unbiased estimation of $F(y^+_{t,i})$, and the same holds for $\bar{f}^-_{t,i}$ and $F(y^-_{t,i})$. As a result, we can analyze the algorithm under the framework of stochastic continuous submodular maximization. By applying Theorem 2, Lemma 3, and the facts $\mathbb{E}[|\bar{f}^+_{t,i} - F(y^+_{t,i})|^2] \leq M^2/S_{t,i}, \mathbb{E}[|\bar{f}^-_{t,i} - F(y^-_{t,i})|^2] \leq M^2/S_{t,i}$ directly, we can also attain Theorem 3.

5 Experiments

In this section, we will compare Black-box Continuous Greedy (BCG) and Discrete Black-box Greedy (DBG) with the following baselines:

(1) Zeroth-Order Gradient Ascent (ZGA) is the projected gradient ascent algorithm equipped with the same two-point gradient estimator as BCG uses. Therefore, it is a *zeroth-order* projected algorithm.

(2) Stochastic Continuous Greedy (SCG) is the state-of-the-art *first-order* algorithm for maximizing continuous DR-submodular functions Mokhtari et al. [2018a,b]. Note that it is a projection-free algorithm.

(3) Gradient Ascent (GA) is the *first-order* projected gradient ascent algorithm Hassani et al. [2017].

The stopping criterion for the algorithms is whenever a given number of iterations is achieved. Moreover, the batch sizes $S_{t,i}$ in Algorithm 1 and B_t in Algorithm 2 are both 1. Therefore, in the experiments, DBG uses 1 query per iteration while SCG uses $\mathcal{O}(d)$ queries.

We perform four sets of experiments which are described in detail in the following. The first two sets of experiments are maximization of continuous DR-submodular functions, which Black-box Continuous Greedy is designed to solve. The last two are submodular set maximization problems. We will apply Discrete Black-box Greedy to solve these problems. The function values at different rounds and the execution times are presented in Fig. 1 and Section 5. The first-order algorithms (SCG and GA) are marked in orange, and the zeroth-order algorithms are marked in blue.

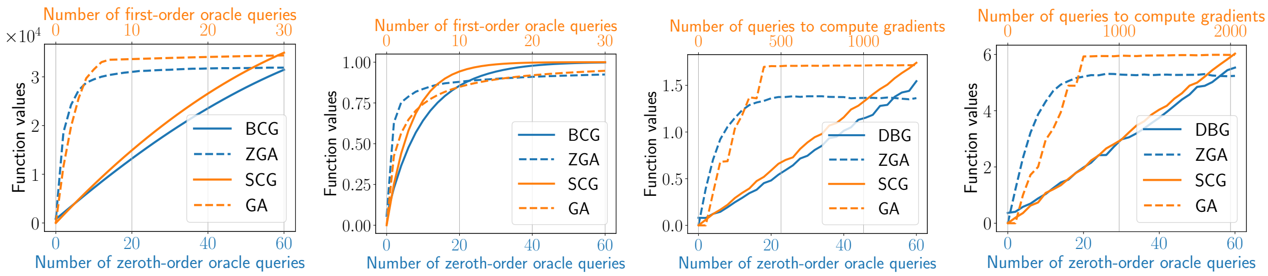
Non-convex/non-concave Quadratic Programming (NQP): In this set of experiments, we apply our proposed algorithm and the baselines to the problem of non-convex/non-concave quadratic programming. The objective function is of the form $F(x) = \frac{1}{2}x^\top Hx + b^\top x$, where x is a 100-dimensional vector, H is a 100-by-100 matrix, and every component of H is an i.i.d. random variable whose distribution is equal to that of the negated absolute value of a standard normal distribution. The constraints are $\sum_{i=1}^{30} x_i \le 30$, $\sum_{i=31}^{60} x_i \le 20$, and $\sum_{i=61}^{100} x_i \le 20$. To guarantee that the gradient is non-negative, we set $b_t = -H^\top \mathbf{1}$. One can observe from Fig. 1a that the function value that BCG attains is only slightly lower than that of the first-order algorithm SCG. The final function value that BCG attains is similar to that of ZGA.

Topic Summarization: Next, we consider the topic summarization problem [El-Arini et al., 2009, Yue and Guestrin, 2011], which is to maximize the probabilistic coverage of selected articles on news topics. Each news article is characterized by its topic distribution, which is obtained by applying latent Dirichlet allocation to the corpus of Reuters-21578, Distribution 1.0. The number of topics is set to 10. We will choose from 120 news articles. The probabilistic coverage of a subset of news articles (denoted by X) is defined by $f(X) = \frac{1}{10}\sum_{j=1}^{10}[1 - \prod_{a\in X}(1 - p_a(j))]$, where $p_a(\cdot)$ is the topic distribution of article a. The multilinear extension function of f is $F(x) = \frac{1}{10}\sum_{j=1}^{10}[1 - \prod_{a\in\Omega}(1 - p_a(j)x_a)]$, where $x \in [0,1]^{120}$ Iyer et al. [2014]. The constraint is $\sum_{i=1}^{40} x_i \le 25$, $\sum_{i=41}^{80} x_i \le 30$, $\sum_{i=81}^{120} x_i \le 35$. It can be observed from Fig. 1b that the proposed BCG algorithm achieves the same function value as the first-ordered algorithm SCG and outperforms the other two. As shown in Fig. 2a, BCG is the most efficient method. The two projection-free algorithms BCG and SCG run faster than the projected methods ZGA and GA. We will elaborate on the running time later in this section.

Active Set Selection We study the active set selection problem that arises in Gaussian process regression Mirzasoleiman et al. [2013]. We use the *Parkinsons Telemonitoring* dataset, which is composed of biomedical voice measurements from people with early-stage Parkinson's disease [Tsanas et al., 2010]. Let $\mathbf{X} \in \mathbb{R}^{n\times d}$ denote the data matrix. Each row $X[i,:]$ is a voice recording while each column $X[:,j]$ denotes an attribute. The covariance matrix Σ is defined by $\Sigma_{ij} = \exp(-\|X[:,i] - X[:,j]\|^2)/h^2$, where h is set to 0.75. The objective function of the active set selection problem is defined by $f(S) = \log\det(I + \Sigma_{S,S})$, where $S \subseteq [d]$ and $\Sigma_{S,S}$ is the principal submatrix indexed by S. The total number of 22 attributes are partitioned into 5 disjoint subsets with sizes 4, 4, 4, 5 and 5, respectively. The problem is subject to a partition matroid requiring that at most one attribute should be active within each subset. Since this is a submodular set maximization problem, in order to evaluate the gradient (i.e., obtain an unbiased estimate of gradient) required by first-order algorithms SCG and GA, it needs $2d$ function value queries. To be precise, the i-th component of gradient is $\mathbb{E}_{S\sim x}[f(S\cup\{i\}) - f(S)]$ and requires two function value queries. It can be observed from Fig. 1c that DBG outperforms the other zeroth-order algorithm ZGA. Although its performance is slightly worse than the two first-order algorithms SCG and GA, it require significantly less number of function value queries than the other two first-order methods (as discussed above).

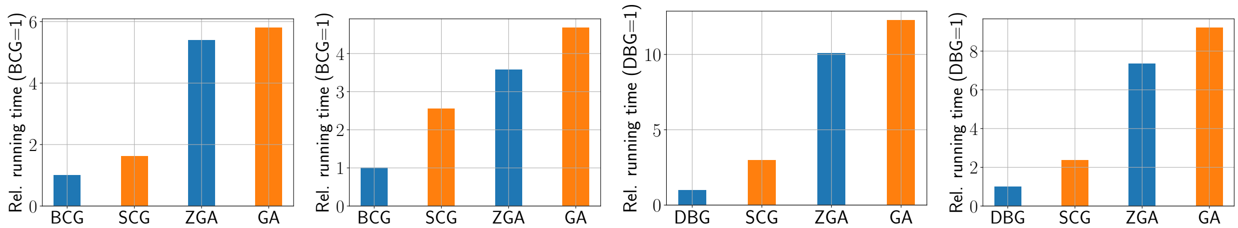
Influence Maximization In the influence maximization problem, we assume that every node in the network is able to influence all of its one-hop neighbors. The objective of influence maximization is to select a subset of nodes in the network, called the seed set (and denoted by S), so that the total number of influenced nodes, including the seed nodes, is maximized. We choose the social network of Zachary's karate club Zachary [1977] in this study. The subjects in this social network are partitioned into three disjoint groups, whose sizes are 10, 14, and 10 respectively. The chosen seed nodes should be subject to a partition matroid; i.e., We will select at most two subjects from each of the three groups. Note that this problem is also a submodular set maximization problem. Similar to the situation in the active set selection problem, first-order algorithms need function value queries to obtain an unbiased estimate of gradient. We can observe from Fig. 1d that DBG attains a better influence coverage than the other zeroth-order algorithm ZGA. Again, even though SCG and GA achieve a slightly better coverage, due to their first-order nature, they require a significantly larger number of function value queries.

Running Time The running times of the our proposed algorithms and the baselines are presented in Section 5 for the above-mentioned experimental setups. There are two main conclusions. First, the two projection-based algorithms (ZGA and GA) require significantly higher time complexity compared to the projection-free algorithms (BCG, DBG, and SCG), as the projection-based algorithms require solving quadratic optimization problems whereas projection-free ones require solving linear optimization problems which can be solved more efficiently. Second, when we compare first-order and zeroth-order algorithms, we



(a) NQP (b) Topic summarization (c) Active set selection (d) Influence maximization

Figure 1: Function value vs. number of oracle queries. Note that every chart has dual horizontal axes. Orange lines use the orange horizontal axes above while blue lines use the blue ones below.



(a) NQP (b) Topic summarization (c) Active set selection (d) Influence maximization

Figure 2: Relative running time normalized with respect to BCG (for continuous DR-submodular maximization in the first two sets of experiments) and DBG (for submodular set maximization in the last two sets of experiments).

can observe that zeroth-order algorithms (BCG, DBG, and ZGA) run faster than their first-order counterparts (SCG and GA).

Summary The above experiment results show the following major advantages of our method over the baselines including SCG and ZGA.

1. BCG/DBG is at least twice faster than SCG and ZGA in all tasks in terms of running time (Figs. 2a to 2d)
2. DBG requires remarkably fewer function evaluations in the discrete setting (Figs. 1c and 1d)
3. In addition to saving function evaluations, BCG/DBG achieves an objective function value comparable to that of the first-order baselines SCG and GA.

Furthermore, we note that the number of first-order queries required by SCG is only half the number required by BCG. However, as is shown in Figs. 2a and 2b, BCG runs significantly faster than SCG since a zeroth-order evaluation is faster than a first-order one.

In the topic summarization task (Fig. 1b), BCG exhibits a similar performance to that of the first-order baselines SCG and GA, in terms of the attained objective function value. In the other three tasks, BCG/DBG runs notably faster while achieving an only slightly inferior function value. Therefore, BCG/DBG is particularly preferable in a large-scale machine learning task and an application where the total number of function evaluations or the running time is subject to a budget.

6 Conclusion

In this paper, we presented Black-box Continuous Greedy, a derivative-free and projection-free algorithm for maximizing a monotone and continuous DR-submodular function subject to a general convex body constraint. We showed that Black-box Continuous Greedy achieves the tight $[(1-1/e)OPT-\epsilon]$ approximation guarantee with $\mathcal{O}(d/\epsilon^3)$ function evaluations. We then extended the algorithm to the stochastic continuous setting and the discrete submodular maximization problem. Our experiments on both synthetic and real data validated the performance of our proposed algorithms. In particular, we observed that Black-box Continuous Greedy practically achieves the same utility as Continuous Greedy while being way more efficient in terms of number of function evaluations.

Acknowledgements

LC is supported by the Google PhD Fellowship. HH is supported by AFOSR Award 19RT0726, NSF HDR TRIPODS award 1934876, NSF award CPS-1837253, NSF award CIF-1910056, and NSF CAREER award CIF-1943064. AK is partially supported by NSF

(IIS-1845032), ONR (N00014-19-1-2406), and AFOSR (FA9550-18-1-0160).

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