Differentiable Greedy Submodular Maximization: Guarantees, Gradient Estimators, and Applications

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Abstract

We consider making outputs of the greedy algorithm for monotone submodular function maximization differentiable w.r.t. parameters of objective functions; this is motivated by many applications, e.g., sensitivity analysis and end-to-end learning. Our contribution is a theoretically guaranteed and widely applicable smoothing framework based on randomization. We prove that our smoothed greedy algorithm almost recovers original approximation guarantees in expectation for the cases of cardinality and \( \kappa \)-extensible system constrains. We also show how to efficiently compute unbiased gradient estimators of any expected output-dependent quantities by sampling outputs. We demonstrate the utility and effectiveness of our framework by applying it to various situations including the aforementioned ones.

1 Introduction

Submodular function maximization is ubiquitous in practice. In many applications such as budget allocation [2], data summarization [35], and active learning [52], submodular functions are modeled with parameters. Formally, we consider the following parametric submodular maximization:

\[
\max_{X \subseteq V} f(X, \theta) \quad \text{subject to} \quad X \in \mathcal{I},
\]

where \( V \) is a set of \( n \) elements, \( f(\cdot, \theta) : 2^V \to \mathbb{R} \) is a set function with continuous-valued parameter vector \( \theta \in \Theta \), and \( \mathcal{I} \subseteq 2^V \) is a set family consisting of all feasible solutions. As is often the case, we assume \( f(\cdot, \theta) \) to be normalized, monotone, and submodular for any \( \theta \in \Theta \) (see, Section 1.2).

Once \( \theta \) is fixed, we often use the greedy algorithm since it has strong theoretical guarantees and delivers high empirical performances. However, if \( \theta \) largely deviates from true unknown \( \hat{\theta} \), the greedy algorithm may output poor solutions to the problem of maximizing \( f(\cdot, \hat{\theta}) \). This naturally raises the following questions. How do changes in \( \theta \) values affect outputs of the greedy algorithm? Can we learn \( \theta \) from data so that the greedy algorithm outputs a good solution for maximizing \( f(\cdot, \hat{\theta}) \)?

In some cases of parametric continuous optimization, we can address those questions by differentiating outputs of algorithms w.r.t. \( \theta \). Such approaches have been studied in the field of sensitivity analysis [43, 18], and those are recently used by decision-focused (or end-to-end) learning methods [14, 53], which learn to predict parameter values based on outputs of optimization algorithms. When it comes to the greedy algorithm for submodular maximization, however, its outputs are not differentiable since continuous changes in \( \theta \) values cause discrete changes in outputs. Therefore, we must use some smoothing techniques for utilizing those well-established methods based on differentiation of outputs.

Tschiatschek et al. [48] opened the field of differentiable greedy submodular maximization; they considered monotone and non-monotone objectives. Their algorithm for monotone objectives was obtained by replacing non-differentiable \( \arg\max \) with differentiable \( \text{softmax} \). They focused on the
We establish a randomization framework for obtaining smoothed greedy algorithms with theoretical guarantees. Although their analysis focuses on the cardinality constrained case. Note that our method is also different from theirs; this result holds if \( \kappa \) belongs to a more general class called the \( \kappa \)-system, which includes \( \kappa \)-extensible systems.

Differentiable greedy submodular maximization algorithms are studied in [48, 42]. Their theoretical results are more limited than ours as explained above. Moreover, their methods are not applicable to our setting: while they differentiate some functions defined with subsets \( X_1, X_2, \ldots \subseteq V \) given as datasets, we aim to differentiate expected output-dependent quantities defined without such subsets (see, Appendix A). Probably, the closest to our result is that of Wilder et al. [53], while their approach is different from ours. They use a continuous relaxation (multilinear extension [10]) of \( f(\cdot, \theta) \) and differentiate its local optimum computed with the stochastic gradient ascent method (SGA) [26], which achieves a 1/2-approximation. Although their method can be applied to matroid constraints, their analysis focuses on the cardinality constrained case. Note that our method is also different from submodular-function learning methods based on samples of \( (X, f(X, \theta)) \) pairs [4, 44].

Differentiable end-to-end learning has been studied in many other settings: submodular minimization [11], quadratic programming [3], mixed integer programming [16], optimization on graphs [54], combinatorial linear optimization [41], and satisfiability (SAT) instances [51].

Stochastic perturbation is an effective smoothing technique used in many situations: linear contextual bandit [30], linear optimization [7], and sampling from discrete distribution [23, 27, 33]. The design of SMOOTHED GREEDY is related to the link between regularization and perturbation (see, e.g., [1]).

Can we smooth the greedy algorithm without losing its theoretical guarantees?

Can we efficiently differentiate outputs of the smoothed greedy algorithm?

We establish a randomization framework for obtaining smoothed greedy algorithms with theoretical guarantees and computing unbiased estimators of derivatives. Our framework is flexible and can serve as a bridge between the combinatorial greedy algorithm and continuous differentiation-based methods in many applications. Below we detail our contributions.

**SMOOTHED GREEDY** We develop SMOOTHED GREEDY by stochastically perturbing \( \arg\max \); this generalizes the algorithms of [48, 42]. We prove that the perturbation does not spoil the original guarantees: almost \( (1 - 1/\epsilon) \)- and \( \frac{1}{\kappa+1} \)-approximation guarantees are achieved in expectation for the cases of cardinality and \( \kappa \)-extensible system constraints, respectively, where a subtractive term depending on the perturbation strength affects the guarantees.

**Gradient estimation** Owing to perturbation, we can differentiate expected outputs of SMOOTHED GREEDY; the computation cost is, however, exponential in \( n \) as with [48]. To circumvent this, we show how to compute unbiased gradient estimators of any expected output-dependent quantities by sampling SMOOTHED GREEDY outputs. This enables us to efficiently estimate derivatives of, e.g., expected objective values and the probability that each \( v \in V \) is chosen.

**Applications** We demonstrate the usefulness of our framework by instantiating it for various settings including sensitivity analysis and decision-focused learning. When applied to sensitivity analysis, it elucidates how SMOOTHED GREEDY can be affected by changes in \( \theta \) values. Results of decision-focused learning experiments suggest that our greedy-based approach can be a simple and effective alternative to a recent continuous relaxation method [53].

## 1.1 Related work

Nemhauser et al. [38] proved the \( (1 - 1/\epsilon) \)-approximation guarantee of the greedy algorithm for the cardinality constrained case, and this result is known to be optimal [37, 15]. Fisher et al. [17] proved that the greedy algorithm achieves the \( \frac{1}{\kappa+1} \)-approximation if \( (V, I) \) is an intersection of \( \kappa \) matroids. Calinescu et al. [10] showed that this result holds if \( (V, I) \) belongs to a more general class called the \( \kappa \)-system, which includes \( \kappa \)-extensible systems.

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Algorithm 1

\( S \)

\( k \) = 1, 2, ... do

3: \( U_k = \{ u_1, \ldots, u_{n_k} \} \leftarrow \{ v \notin S \mid S \cup \{ v \} \in \mathcal{I} \} \)

4: \( g_k(\theta) = (g_k(u_1, \theta), \ldots, g_k(u_{n_k}, \theta)) \leftarrow (f_S(u_1, \theta), \ldots, f_S(u_{n_k}, \theta)) \)

5: \( p_k(\theta) = (p_k(u_1, \theta), \ldots, p_k(u_{n_k}, \theta)) \leftarrow \arg\max_{p \in \Delta^{n_k}} \{ g_k(\theta), p \} - \Omega_k(p) \}

6: \( s_k \leftarrow u \in U_k \) with probability \( p_k(u, \theta) \)

7: \( S \leftarrow S \cup \{ s_k \} \)

8: if \( S \) is maximal then return \( S \)

1.2 Notation and definition

For any set function \( f : 2^V \rightarrow \mathbb{R} \), we define \( f_X(Y) := f(X \cup Y) - f(X) \). We say \( f \) is normalized if \( f(\emptyset) = 0 \), monotone if \( X \subseteq Y \) implies \( f(X) \leq f(Y) \), and submodular if \( f_X(v) \geq f_Y(v) \) for all \( X \subseteq Y \) and \( v \notin Y \). In this paper, we assume the objective function, \( f(\cdot, \theta) \), to be normalized, monotone, and submodular for any \( \theta \in \Theta \). Note that this is the case with many submodular functions, e.g., weighted coverage functions with non-negative weights \( \theta \), probabilistic coverage functions with probabilities \( \theta \), and deep submodular functions [12] with non-negative linear-layer weights \( \theta \).

We say \((V, \mathcal{I})\) is a \( \kappa \)-extensible system [34] if the following three conditions hold: (1) \( \emptyset \in \mathcal{I} \), (2) \( X \subseteq Y \in \mathcal{I} \) implies \( X \in \mathcal{I} \), and (3) for all \( X, Y \in \mathcal{I} \) and \( v \notin X \) such that \( X \cup \{ v \} \in \mathcal{I} \), and for every \( Y \supset X \) such that \( Y \in \mathcal{I} \), there exists \( Z \subseteq Y \setminus X \) that satisfies \( |Z| \leq \kappa \) and \( Y \setminus \{ v \} \in \mathcal{I} \). We say \( X \in \mathcal{I} \) is maximal if no \( Y \in \mathcal{I} \) strictly includes \( X \). As shown in [34], \((V, \mathcal{I})\) is a matroid iff it is a 1-extensible system, which includes the case of cardinality constraints as a special case, and the intersection of \( \kappa \) matroids defined on a common ground set always forms a \( \kappa \)-extensible system. We define \( K := \max_{X \in \mathcal{I}} |X| \), which is so-called the rank of \((V, \mathcal{I})\).

For any positive integer \( n \), we let \( 0_n \) and \( 1_n \) be \( n \)-dimensional all-zero and all-one vectors, respectively. For any finite set \( V \) and \( S \subseteq V \), we let \( 1_S \in \mathbb{R}^{|V|} \) denote the indicator vector of \( S \); i.e., the entries corresponding to \( S \) are 1 and the others are 0. Given any scalar- or vector-valued differentiable function \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \), \( \nabla_x f(x) \in \mathbb{R}^{m \times n} \) denotes its gradient or Jacobian, respectively.

2 Smoothed greedy algorithm

We present SMOOTHED GREEDY and prove its approximation guarantees. In this section, we take parameter \( \theta \in \Theta \) to be fixed arbitrarily.

Algorithm 1 is the details of SMOOTHED GREEDY. In the \( k \)-th iteration, we compute marginal gains \( f_S(u, \theta) \) of all addable elements \( u \in U_k := \{ v \notin S \mid S \cup \{ v \} \in \mathcal{I} \} \), which we index as \( u_1, \ldots, u_{n_k} \) for convenience (\( n_k \leq n \)). Let \( g_k(\theta) \in \mathbb{R}^{n_k} \) denote the marginal gain vector. We then compute

\[
\begin{align*}
p_k(\theta) &= \arg\max_{p \in \Delta^{n_k}} \{ g_k(\theta), p \} - \Omega_k(p),
\end{align*}
\]

where \( \Delta^{n_k} := \{ x \in \mathbb{R}^{n_k} \mid 0_{n_k} \leq x \leq 1_{n_k}, \langle x, 1_{n_k} \rangle = 1 \} \) is the \( n_k \)-dimensional probability simplex and \( \Omega_k : \mathbb{R}^{n_k} \rightarrow \mathbb{R} \) is a strictly convex function; we call \( \Omega_k \) a regularization function. Note that the strict convexity implies the uniqueness of \( p_k(\theta) \). We then choose an element, \( u \in U_k \), with probability \( p_k(u, \theta) \); let \( s_k \) be the chosen element. This procedure can be seen as a stochastically perturbed version of \( \arg\max \); without \( \Omega_k \), we have \( s_k \in \arg\max_{u \in U_k} f_S(u, \theta) \). We make a remark about the notation, \( p_k(\theta) \). Since \( p_k(\theta) \) depends on \( f_S(u, \theta) \) where \( S = \{ s_1, \ldots, s_{k-1} \} \), it should be denoted by, e.g., \( p_k(\theta, s_1, \ldots, s_{k-1}) \). We however omit \( s_1, \ldots, s_{k-1} \) for simplicity; the dependence on \( s_1, \ldots, s_{k-1} \) will be clear from the context.

Let \( \delta \geq 0 \) be a constant such that, for every \( k \) and any \( p, q \in \Delta^{n_k}, \delta \geq \Omega_k(p) - \Omega_k(q) \) holds. As shown in Theorems 1 and 2, smaller \( \delta \) values yield better guarantees. Below we present examples of \( \Omega_k \) and their \( \delta \) values.

Entropy function Let \( \Omega_k(p) = \epsilon \sum_{i=1}^{n_k} p(u_i) \ln p(u_i) \), where \( p(u_i) \) is the \( i \)-th entry of \( p \in \mathbb{R}^{n_k} \) and \( \epsilon > 0 \) is an arbitrary constant. In this case, we have \( \delta = \epsilon \ln n_k \), and thus we can make the \( \delta \) value arbitrarily small by controlling the \( \epsilon \) value. In this case, Steps 4–6 can be efficiently performed via softmax sampling as with \([48, 42]\); i.e., \( p_k(u, \theta) \propto \exp(f_S(u, \theta)/\epsilon) \) (see, Appendix C.1).
Quadratic function We can use strongly convex quadratic functions as $\Omega_k$. To be specific, if we let $\Omega_k(p) = \epsilon \|p\|_2^2$, then $\delta = \epsilon (1 - 1/n_k) \leq \epsilon$. In this case, we need to solve quadratic programming (QP) problems for $k = 1, 2, \ldots$. If we use the same $\Omega_k$ for every $k$, preconditioning (e.g., decomposition of Hessian matrices) is effective. We can also use an efficient batch QP solver [3].

As above, the $\delta$ value is typically controllable and plays a role as a hyper-parameter that balances the trade-off between the approximation guarantees and smoothness; how to set the $\delta$ value should be discussed depending on applications (see, Section 4). We can also use other strictly convex functions, such as the convex combination of the above two functions. When differentiating outputs of SMOOTHED GREEDY, we need an additional assumption on $\Omega_k$ (see, Assumption 2 in Section 3).

Below we present the approximation guarantees (see, Appendix B for proofs). As is often the case with analyses of the greedy algorithm, we begin by lower bounding the expected marginal gain.

**Lemma 1.** In any $k$-th step, conditioned on the $(k-1)$-th step (i.e., $S = \{s_1, \ldots, s_{k-1}\}$ is arbitrarily fixed), we have $E[f_S(s_k, \theta)] \geq f_S(u, \theta) - \delta$ for any $u \in U_k$.

Lemma 1 enables us to utilize analysis techniques for the greedy algorithm. Let $S$ and $O$ be an output of Algorithm 1 and a maximal optimal solution to problem (1), respectively. In the cardinality constrained case, the following theorem holds.

**Theorem 1.** If $T = \{X \subseteq V \mid |X| \leq K\}$, we have $E[f(S, \theta)] \geq (1 - 1/e)f(O, \theta) - \delta K$.

In the case of $\kappa$-extensible systems, we can prove the deterministic greedy algorithm, to our stochastic SMOOTHED GREEDY.

**Theorem 2.** If $(V, T)$ is a $\kappa$-extensible system with rank $K$, we have $E[f(S, \theta)] \geq \frac{1}{\kappa+1} f(O, \theta) - \delta K$.

Proof sketch of Theorem 2. The $\frac{1}{\kappa+1}$-approximation guarantee of the deterministic greedy algorithm can be proved as follows. For a series of subsets $\emptyset = S_0 \subseteq S_1 \subseteq \cdots \subseteq S_{|S|} = S$ obtained in $|S|$ steps of the greedy algorithm, we construct a series of subsets $O = O_0, O_1, \ldots, O_{|S|} = S$ that satisfies $S_i \subseteq O_i \in T$ and $\kappa \cdot (f(S_i, \theta) - f(S_{i-1}, \theta)) \geq f(O_{i-1}, \theta) - f(O_i, \theta)$ for $i = 1, \ldots, |S|$. The $\frac{1}{\kappa+1}$-approximation is obtained by summing both sides of the inequality for $i = 1, \ldots, |S|$. In our proof, we show that such $O_0, O_1, \ldots$ can be constructed for each realization of the randomness of SMOOTHED GREEDY, and we prove

$$\kappa \cdot \left( E[f(S_i, \theta)] - E[f(S_{i-1}, \theta)] \right) + \delta \geq E[f(O_{i-1}, \theta)] - E[f(O_i, \theta)]$$

for $i = 1, \ldots, K$ by using Lemma 1, where we must carefully deal with the fact that $|S|$ is not always equal to $K$. We obtain Theorem 2 by summing both sides of the inequality for $i = 1, \ldots, K$.

3 Gradient estimation

We discusses how to differentiate outputs of SMOOTHED GREEDY w.r.t. $\theta$. In this section, we assume the following two differentiability conditions to hold:

**Assumption 1.** For any $X \subseteq V$, we assume $f(X, \theta)$ to be differentiable w.r.t. $\theta$.

**Assumption 2.** For any $\theta \in \Theta$ and $k \in \{1, \ldots, K\}$, let $p_k(g_k, \theta)$ be the maximizer, $p_k(\theta)$, of (2) regarded as a function of $g_k(\theta)$. We assume $p_k(g_k)$ to be differentiable w.r.t. $g_k$.

Assumption 1 is inevitable; the existing studies [48, 42, 53] are also based on this condition. Examples of functions satisfying Assumption 1 include weighted coverage functions (w.r.t. weights of covered vertices), probabilistic coverage functions [53], and deep submodular functions with smooth activation functions [12]. At the end of this section, we discuss what occurs if Assumption 1 does not hold and possible remedies for addressing such cases in practice.

Assumption 2 can be satisfied by appropriately designing $\Omega_k$. If $\Omega_k$ is the entropy function, the $i$-th entry of $p_k(g_k)$ can be written as $\exp(\epsilon^{-1} g_k(u_i, \theta)) / \sum_{u \in U_k} \exp(\epsilon^{-1} g_k(u, \theta))$; hence $p_k(g_k)$ is differentiable w.r.t. $g_k$. If we use strongly convex quadratic functions as $\Omega_k$, the differentiability condition holds if the strict complementarity is satisfied at $p_k(\theta)$ (see, [3]). In Appendix C.2, we present a sufficient condition for $\Omega_k$ to satisfy Assumption 2.

We then introduce the probability distribution of SMOOTHED GREEDY outputs, which we call the output distribution for convenience. This is useful for clearly describing our method. Although a similar notion is considered in [48], our way of using it is quite different (see, Appendix A).
Definition 1 (Output distribution). Let $\mathcal{S}_{\leq K}$ denote the set of all sequences consisting of at most $K$ elements in $V$. For any fixed $\theta$, we define $p(\theta) : \mathcal{S}_{\leq K} \rightarrow [0, 1]$ as the probability distribution function of SMOOTHED GREEDY outputs, i.e., $S \sim p(\theta)$. We call $p(\theta)$ the output distribution. We use $p(S, \theta) \in [0, 1]$ to denote the probability that $S \in \mathcal{S}_{\leq K}$ is returned by SMOOTHED GREEDY.

For example, if $V = \{1, 2, 3\}$, then $\mathcal{S}_{\leq 2}$ consists of $(\), (1), (2), (3), (1, 2), (1, 3), (2, 1), (3, 2),$ and $(3, 1)$. Note that for a sequence $S = (s_1, \ldots, s_{|S|})$ constructed by SMOOTHED GREEDY, we have $p(S, \theta) = \prod_{k=1}^{|S|} p_k(s_k, \theta)$, where $p_k(s_k, \theta)$ is the entry of $p_k(\theta)$ corresponding to $s_k \in U_k$.

We now aim to compute $\nabla \theta \mathbb{E}_{S \sim p(\theta)}[Q(S)] = \Sigma_{S \in \mathcal{S}_{\leq K}} Q(S) \nabla \theta p(S, \theta)$, where $Q(S)$ is any scalar or vector-valued quantity; we present examples of $Q(S)$ in Section 4. Since the size of $\mathcal{S}_{\leq K}$ is exponential in $K = O(n)$, we usually cannot compute the exact derivative in practice. We circumvent the exponential computation cost by instead using the score-function gradient estimator [45] (a.k.a. the likelihood estimator [20] and REINFORCE [55]). Specifically, since we have

$$\nabla \theta \mathbb{E}_{S \sim p(\theta)}[Q(S)] = \Sigma_{S \in \mathcal{S}_{\leq K}} Q(S) \nabla \theta \ln p(S, \theta) = \mathbb{E}_{S \sim p(\theta)}[Q(S) \nabla \theta \ln p(S, \theta)],$$

we can compute an unbiased gradient estimator by sampling $N$ outputs of SMOOTHED GREEDY (regarded as sequences) as follows:

$$\frac{1}{N} \sum_{j=1}^{N} Q(S_j) \nabla \theta \ln p(S_j, \theta) \quad \text{where} \quad S_j \sim p(\theta).$$

The remaining problem is how to compute $\nabla \theta \ln p(S, \theta)$ for sampled sequence $S = (s_1, \ldots, s_{|S|})$. Note that since we have

$$\nabla \theta \ln p(S, \theta) = \nabla \theta \ln \prod_{k=1}^{|S|} p_k(s_k, \theta) = \sum_{k=1}^{|S|} \frac{1}{p_k(s_k, \theta)} \nabla \theta p_k(s_k, \theta),$$

it suffices to compute $\nabla \theta p_k(s_k, \theta)$ for $k \in \{1, \ldots, |S|\}$. From Assumptions 1 and 2, we can differentiate $p_k(\theta)$ by using the chain rule as $\nabla \theta p_k(\theta) = \nabla g_k p_k(\theta) \cdot \nabla \theta g_k(\theta)$; the row corresponding to $s_k \in U_k$ is equal to $\nabla \theta p_k(s_k, \theta)$. In some cases where we can analytically express $p_k(\theta)$ as a simple function of $\theta$, we can directly compute $\nabla \theta \ln p(S, \theta)$ via automatic differentiation [39, 6].

Other than the score function method, there are several major gradient estimation methods (see, [36]). In Appendix D, we discuss why it is difficult to apply those methods to our setting.

Variance reduction In practice, the variance of the gradient estimators can be excessive, which requires us to sample too many outputs of SMOOTHED GREEDY. Fortunately, there are various methods for reducing the variance of such Monte Carlo gradient estimators [21, 49, 36]. A simple and popular method is the following baseline correction [55]: we use $Q(S) - \beta$ instead of $Q(S)$, where $\beta$ is some coefficient. If $\beta$ is a constant, the estimator remains unbiased since $\mathbb{E}_{S \sim p(\theta)}[\nabla \theta \ln p(S, \theta)] = \nabla \theta \mathbb{E}_{S \sim p(\theta)}[1] = 0$. By optimizing $\beta$, we can reduce the variance. In practice, $\beta$ is often estimated with the running average of $Q(\cdot)$ values, which we use in the experiments (Section 5).

Non-differentiable cases If Assumption 1 does not hold, i.e., $f(X, \theta)$ is non-differentiable w.r.t. $\theta$, the above discussion is incorrect because the chain rule fails to hold [22]. This issue is common with many machine learning scenarios, e.g., training of NNs with ReLU activation functions. The current state of affairs is that we disregard the issue since it rarely brings harm in practice. Recently, Kakade and Lee [28] developed a subdifferentiation method for addressing such non-differentiable cases; this result may enable our method to deal with non-differentiable $f(X, \theta)$.

4 Applications

Our framework has many potential applications owing to its flexibility and simplicity. We here show how to use it for sensitivity analysis and decision-focused learning settings. In Appendix E, we discuss other applications related to learning of submodular models with oracle queries.
4.1 Sensitivity analysis

When addressing parametric optimization instances, the sensitivity—how and how much changes in parameter values can affect outputs of algorithms—is our major concern, and hence widely studied. In continuous optimization settings, most methods are based on differentiation [43, 18, 8]. In contrast, sensitivity analysis methods for combinatorial settings are diverse [24, 9, 19, 50] probably due to the non-differentiability; the score function method is also used for analyzing the sensitivity of discrete systems (e.g., querying systems) [31]. As explained below, our gradient estimation method can be used for analyzing the sensitivity of SMOOTHED GREEDY, which can become arbitrarily close to the greedy algorithm by controlling the δ value. To the best of our knowledge, this provides the first method for analyzing the sensitivity of the greedy algorithm for submodular maximization.

We analyze the sensitivity of the probability that each v ∈ V is included in an output of SMOOTHED GREEDY, which can be expressed as E_{S \sim p(\theta)}[1_S] = \Sigma_{S \in \mathcal{F} \subset K} 1_S p(S, \theta). By using our method in Section 3 with Q(S) = 1_S, we can estimate the Jacobian matrix as

$$\nabla_\theta E_{S \sim p(\theta)}[1_S] \approx \frac{1}{N} \sum_{j=1}^{N} 1_{S_j} \nabla_\theta \ln p(S_j, \theta).$$

Here, given any \( \theta \), the \((v, j)\) entry of the Jacobian matrix represents how and how much the infinitesimal increase in the \( j \)-th entry of \( \theta \) affects the probability that \( v \in V \) is chosen; i.e., how sensitive each \( v \in V \) is to uncertainties in \( \theta \) values. This information will be beneficial to practitioners who address tasks involving submodular maximization with uncertain parameters; for example, advertisers who want to know reliable ways to promote products (we will further discuss this in Broader Impact section). An experiment in Section 5.1 demonstrates how our sensitivity analysis method works.

4.2 Decision-focused learning

We consider a situation where \( \theta \) is computed with some predictive models (e.g., NNs). Let \( m(\cdot, w) \) be a predictive model that maps some observed feature \( X \) to \( \theta \), where \( w \) represents model parameters. We train \( m(\cdot, w) \) by optimizing \( w \) values with training datasets \((X_1, \theta_1), \ldots, (X_M, \theta_M)\). Given test instance \((X, \hat{\theta})\), where \( \hat{\theta} \) is the true unknown parameter, the trained model predicts \( \theta = m(X, w) \), and we obtain solution \( S \) (or, make a decision) by approximately maximizing \( f(\cdot, \theta) \). Our utility (decision quality) is given by \( f(S, \theta) \). For example, in the case of influence maximization on a network, \( \theta \) represents link probabilities, which are computed by \( m(\cdot, w) \) for observed feature \( X \). We make a decision by activating nodes in \( S \). Our utility is the influence spread measured by \( f(S, \theta) \), where \( \hat{\theta} \) represents unknown true link probabilities.

With the decision-focused learning methods [14, 53], we train predictive models in an attempt to maximize the decision quality, \( f(S, \hat{\theta}) \). This approach is empirically more effective for the above setting involving both prediction and optimization than the standard two-stage approach, which trains models with some predetermined loss functions and then make decisions. By combining our framework with the decision-focused approach, we can train predictive models with first-order methods so that expected objective values achieved by SMOOTHED GREEDY become large.

Below we present a specific training procedure with our framework and stochastic first-order methods. We aim to minimize the empirical loss function expressed as \(-\frac{1}{M} \Sigma_{i=1}^{M} E_{S \sim p(m(X_i, w))}[f(S, \theta_i)]\), where \( p(\cdot) \) is the output distribution. In each iteration, we sample a training dataset, \((X_i, \theta_i)\), and compute \( \theta = m(X_i, w) \) with the current \( w \) values. We then perform \( N \) trials of SMOOTHED GREEDY to estimate the current loss function value, \(-E_{S \sim p(\theta)}[f(S, \theta)]\). Next, we estimate the gradient by using our method with \( Q(S) = f(S, \theta_i) \). More precisely, for each \( j \)-th trial of SMOOTHED GREEDY, we compute \( \nabla_\theta \ln p(S_j, \theta) \) as explained in Section 3 and estimate the gradient as follows:

$$-\nabla_w E_{S \sim p(m(X_i, w))}[f(S, \theta_i)] \approx -\frac{1}{N} \Sigma_{j=1}^{N} f(S_j, \theta_i) \nabla_\theta \ln p(S_j, \theta)|_{\theta = m(X_i, w)} \cdot \nabla_w m(X_i, w).$$

We update \( w \) by using the above gradient estimator. When using mini-batch update methods, we compute the above gradient estimator over a batch of datasets and update \( w \). If \( m \) is not differentiable, the above chain rule fails to hold, but we can often disregard this in practice as discussed in Section 3.
We use Algorithm 1, we use $\Omega_k(p) = \epsilon \sum_{u \in U_k} p(u) \ln p(u)$ with $\epsilon = 0.2$.

We use bipartite influence maximization instances described as follows. Let $V$ and $T$ be sets of items and targets, respectively, and $\theta \in [0, 1]^{V \times T}$ be link probabilities. We aim to maximize the expected number of influenced targets, $f(X, \theta) = \sum_{t \in T} \left(1 - \prod_{v \in X} (1 - \theta_{v,t})\right)$, by choosing up to $K$ items.

We present additional experiments in Appendix E.2, where we consider maximizing deep submodular functions under matroid constraints.

5 Experiments

We evaluate our method with sensitivity analysis and decision-focused learning instances. We use a 64-bit macOS machine with 1.6GHz Intel Core i5 CPUs and 16GB RAMs. As a regularization function of Algorithm 1, we use $\Omega_k(p) = \epsilon \sum_{u \in U_k} p(u) \ln p(u)$ with $\epsilon = 0.2$.

We use bipartite influence maximization instances described as follows. Let $V$ and $T$ be sets of items and targets, respectively, and $\theta \in [0, 1]^{V \times T}$ be link probabilities. We aim to maximize the expected number of influenced targets, $f(X, \theta) = \sum_{t \in T} \left(1 - \prod_{v \in X} (1 - \theta_{v,t})\right)$, by choosing up to $K$ items.

We present additional experiments in Appendix E.2, where we consider maximizing deep submodular functions under matroid constraints.

5.1 Sensitivity analysis

We perform sensitivity analysis on a synthetic instance with $V = \{v_1, v_2, v_3\}$, $T = \{t_1, t_2, t_3\}$, and $K = 2$. Let $\theta_{i,j}$ denote the link probability of $(v_i, t_j)$; we set $(\theta_{1,1}, \theta_{1,2}, \theta_{1,3}) = (0.4, 0.4, 0)$, $(\theta_{2,1}, \theta_{2,2}, \theta_{2,3}) = (0, 0.4, 0.2)$, and $(\theta_{3,1}, \theta_{3,2}, \theta_{3,3}) = (0, 0, 0.2)$ as in Figure 1a. We analyze the sensitivity of SMOOTHED GREEDY outputs by estimating $\nabla_{\theta} E_{S \sim p(\theta)}[1_S]$ as explained in Section 4.1.

We let $N = 100$ and use the baseline correction method (see, Section 5) to reduce the variance.

Figures 1b, 1c, and 1d illustrate how and how much the increase in each $\theta_{i,j}$ value can affect the probability that $v_1$, $v_2$, and $v_3$, respectively, are chosen. In this setting, the objective values of the three maximal solutions, $\{v_1, v_2\}$, $\{v_1, v_3\}$, and $\{v_2, v_3\}$, are 1.24, 1.00, and 0.76, respectively. Therefore, SMOOTHED GREEDY returns $\{v_1, v_2\}$ or $\{v_1, v_3\}$ with a high probability, and this remains true even if $\theta$ values slightly change. Consequently, the probability of choosing $v_1$ is relatively insensitive (see, Figure 1b). In contrast, the probabilities of choosing $v_2$ and $v_3$ are highly sensitive (see, Figures 1c and 1d). For example, if $\theta_{2,3}$ increases, the probability that the algorithm returns $\{v_1, v_2\}$ or $\{v_1, v_3\}$ increases (decreases), which means the probability of choosing $v_2$ ($v_3$) is positively (negatively) affected by the increase in $\theta_{2,3}$. We can also see the that the opposite occurs if $\theta_{3,3}$ increases.

5.2 Decision-focused learning

We evaluate the performance of our method via decision-focused learning experiments with MovieLens 100K dataset [25], which contains 100, 000 ratings (1–5) of 1, 682 movies made by 943 users. We set the link probabilities at 0.02, 0.04, . . . , 0.1 according to the ratings, and those of unrated ones are set at 0. We randomly sample 100 movies and 500 users, which form item set $V$ and target set $T$, respectively; we thus make 100 random $(V, T)$ pairs with link probabilities. Each movie $v \in V$
We compare SG\- with Two-stage algorithms and continuous optimization methods in two settings, each with different learning rates and stopping criteria. These results are consistent with the theoretical guarantees. Namely, while Continuous methods train the model so that the (almost) $1/2$-approximation algorithm, can achieve high objective values, our methods train the model so that the (almost) $(1-1/e)$-approximation (smoothed) greedy algorithm can achieve high objective values. We see that the variance reduction method is effective for improving the performances of our method. The standard deviation of (VR-)SG becomes sometimes high; this is because they are sometimes trapped in poor local optima and result in highly deviated objective values. Considering this, the performance of our method seems to be further improved if it can be combined with NN training techniques for escaping from poor local optima. Regarding running times for updating $w$ on a mini-batch, SG-1 takes 2.81, 3.38, and 3.77 seconds on average for $K = 5, 10$, and 20, respectively, while Continuous takes 5.86, 5.87, and 6.11 seconds. Hence, our methods can run faster by performing Smoothed Greedy in parallel as mentioned in Section 4.1.

Table 1: Function values achieved with each method.

|       | $K = 5$ |       | $K = 10$ |       | $K = 20$ |
|-------|---------|-------|----------|-------|----------|
|       | Training | Test  | Training | Test  | Training | Test  |
| SG-1  | 26.3 ± 4.0 | 26.4 ± 4.4 | 46.0 ± 5.9 | 45.9 ± 6.5 | 69.7 ± 23.8 | 69.6 ± 24.1 |
| SG-10 | 29.0 ± 3.7 | 28.1 ± 4.9 | 47.0 ± 12.1 | 46.1 ± 12.4 | 71.5 ± 28.0 | 70.6 ± 28.1 |
| SG-100| 33.6 ± 2.4 | 32.0 ± 3.8 | 54.3 ± 2.0 | 53.5 ± 4.2 | 82.6 ± 21.8 | 82.3 ± 21.7 |
| VR-SG-10 | 35.2 ± 6.1 | 33.7 ± 6.2 | 57.9 ± 1.6 | 56.2 ± 3.4 | 90.8 ± 16.5 | 89.5 ± 16.7 |
| VR-SG-100 | 36.8 ± 0.9 | 35.6 ± 2.2 | 59.9 ± 1.6 | 58.0 ± 2.9 | 96.8 ± 1.1 | 94.5 ± 2.6 |
| Continuous | 24.0 ± 4.5 | 23.2 ± 4.9 | 43.2 ± 6.1 | 42.3 ± 7.1 | 81.7 ± 6.8 | 81.3 ± 6.6 |
| Two-stage | 17.3 ± 1.2 | 17.3 ± 2.1 | 35.6 ± 0.9 | 35.6 ± 2.7 | 65.5 ± 4.0 | 64.8 ± 5.1 |
| Random   | 17.5 ± 1.0 | 17.6 ± 2.2 | 33.8 ± 0.8 | 34.0 ± 2.7 | 64.0 ± 1.3 | 64.5 ± 2.6 |

We mostly replicate the settings of budget allocation instances in [53], but we use the public MovieLens dataset instead of the original one that is not open to the public; accordingly, some parts are slightly changed.

1 We mostly replicate the settings of budget allocation instances in [53], but we use the public MovieLens dataset instead of the original one that is not open to the public; accordingly, some parts are slightly changed.
Broader Impact

The greedy algorithm for submodular maximization is one of the most attractive topics of combinatorial optimization in the machine learning (ML) community. On the other hand, many recent advances in ML methods are based on continuous optimization; particularly, NNs are mostly trained with stochastic first-order methods. Our work will benefit the optimization and ML communities by bridging the combinatorial greedy algorithm and continuous first-order optimization methods. We present examples of situations where our framework is useful.

Reliability assessment Submodular maximization sometimes appears when making vital decisions: allocation of large resources to advertising channels and placement of sensors for observing important events. In such cases, after obtaining a solution with the greedy algorithm, to assess its reliability—how robust the solution is against uncertainties in parameters of submodular functions—is important. This is possible with the sensitivity analysis method based on our framework (see, Sections 4.1 and 5.1). If we find that the solution is reliable enough, we can put it into practice; otherwise, we can use robust submodular maximization methods (e.g., [46]) to strike a balance between the objective value and robustness. Note that, since outputs of robust optimization algorithms can be pessimistic, assessing the reliability of solutions obtained by the greedy algorithm at first is useful; this approach will be beneficial to many practitioners as mentioned in Section 4.1.

End-to-end learning The combination of our framework and end-to-end learning methods is effective as shown in Sections 4.2 and 5.2; we also discuss analogous settings and present experiments in Appendix E. In practice, this approach is useful particularly when we do not have enough prior knowledge on model structures and the prevalent two-stage methods do not work well. The flexibility and simplicity of our framework can also be practical advantages. For example, we can customize regularization functions for improving empirical performances depending on applications. We also need not consider the multilinear extension of objective functions unlike [54]. Furthermore, in some cases we can easily implement the gradient estimation method by utilizing automatic differentiation packages such as PyTorch [39]; this is possible, for example, if we use the entropy function as $\Omega_k$ and a differentiable deep submodular function as $f(\cdot; \theta)$.

In summary, the positive aspect of our work is that it is useful for developing various practically effective methods.

As a negative aspect, failures of systems that use our method may result in harmful consequences. In particular, when our method is combined with NNs, how to avoid failures (or poor local optima) is an important subject of study as mentioned in Section 5.2. We leave this for future work since it requires application-dependent discussions and goes beyond the scope of this paper.

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Appendix

A Comparisons with existing greedy methods

We provide detailed comparisons of our work and the exiting studies on the differentiable greedy algorithms [48, 42], which use softmax instead of argmax. We clarify the difference in the problem settings, and we also explain that the differentiation methods are completely different.

Tschiatschek et al. [48] consider differentiating the likelihood that measures how an output of their algorithm can be close to $X_1, X_2, \ldots$, which are some good solutions given as datasets. To this end, we need to differentiate $P(X) := \Sigma_{\sigma \in \Sigma(X)} P(\sigma, \theta)$, where $X \in \{X_1, X_2, \ldots\}$ is a given subset, $\Sigma(X)$ is the set of all permutations of elements in $X$, and $P(\sigma, \theta)$ is the probability that their algorithm returns sequence $\sigma \in \mathcal{J}_{\leq \ v}$. Since the computation of the summation over $\Sigma(X)$ is too costly, they employ the following heuristic approximation: if the temperature of softmax is low, we let $P(X) \approx P(\sigma^G, \theta)$, where $\sigma^G$ is obtained by the greedy algorithm, and if the temperature is high, we let $P(X) \approx |X|! \times P(\sigma^K, \theta)$, where $\sigma^K$ is a random permutation. As a result, the computed derivative has no theoretical guarantees unlike our unbiased gradient estimators. Note that our method can provide an unbiased estimator of the desired derivative as follows: we let $Q(S)$ return 1 if $S$ and $X$ consist of the same elements and 0 otherwise, and we estimate $\nabla_\theta \mathbb{E}_{S \sim p(\theta)}[Q(S)]$.

Powers et al. [42] focus on some cases where differentiation can be performed in a more straightforward manner. Specifically, they consider some loss function $L(\ X, p_1(\theta), \ldots, p_K(\theta))$ that is differentiable w.r.t. $p_1(\theta), \ldots, p_K(\theta)$, where $X \subseteq u$ is a given subset. In their setting, $p_1(\theta)$ is the probability distribution vector of softmax and $f(X, \theta)$ is differentiable w.r.t. $\theta$. Therefore, once $X$ is given, $L(\ X, p_1(\theta), \ldots, p_K(\theta))$ can readily be differentiated via automatic differentiation. This setting is completely different from ours; for example, they do not take the randomness of outputs, which are distributed over $\mathcal{J}_{\leq \ v}$, into account.

As described above, both methods are designed for differentiating some functions defined with subsets $X_1, X_2, \ldots$ given as datasets. On the other hand, we do not assume such subsets to be given and consider differentiating the expected value, $\mathbb{E}_{S \sim p(\theta)}[Q(S)]$; this enables us to use our framework for sensitivity analysis and decision-focused learning. The existing methods cannot be used for those applications.

B Proofs of approximation guarantees

In the following analysis, we let $S_k$ denote the solution constructed in the $k$-th step of Algorithm 1; we define $S_0 = \emptyset$. For simplicity, we omit the fixed parameter, $\theta$, in this section. The following discussion holds as long as $f(\cdot, \theta)$ is normalized, monotone, and submodular.

**Lemma 1.** In any $k$-th step, conditioned on the $(k-1)$-th step (i.e., $S = \{s_1, \ldots, s_{k-1}\}$ is arbitrarily fixed), we have $\mathbb{E}[f_S(s_k, \theta)] \geq f_S(u, \theta) - \delta$ for any $u \in U_k$.

**Proof.** From the rule of choosing $s_k$, we have $\mathbb{E}[f_S(s_k)] = \langle g_k, p_k \rangle$. Let $1_u \in \mathbb{R}^n$ be the indicator vector of $u \in U_k$. Since we have $\langle g_k, 1_u \rangle = f_S(u)$ and $1_u \in \Delta^n$, we can obtain the inequality as follows:

$$\mathbb{E}[f_S(s_k)] = \langle g_k, p_k \rangle = \max_{\mathbf{p} \in \Delta^n} \{\langle g_k, \mathbf{p} \rangle - \Omega_k(\mathbf{p})\} + \Omega_k(p_k)$$

$$\geq \langle g_k, 1_u \rangle - (\Omega_k(1_u) - \Omega_k(p_k)) \geq f_S(u) - \delta,$$

where the last inequality comes from $\delta \geq \Omega_k(\mathbf{p}) - \Omega_k(q)$ for any $\mathbf{p}, q \in \Delta^n$.

**Theorem 1.** If $\mathcal{I} = \{X \subseteq u \mid |X| \leq K\}$, we have $\mathbb{E}[f(S, \theta)] \geq (1 - 1/e) f(O, \theta) - \delta K$.

**Proof.** For any $k = 1, \ldots, K$, conditioned on the realization of the $(k-1)$-th step, from Lemma 1 and the submodularity, we obtain

$$\mathbb{E}[f_{S_{k-1}}(s_k)] \geq \frac{1}{K} \sum_{v \in O \setminus S_{k-1}} f_{S_{k-1}}(v) - \delta \geq \frac{1}{K} f_{S_{k-1}}(O) - \delta.$$
By taking expectation over all possible realizations of the \((k-1)\)-th step and using the monotonicity, we obtain
\[
E[f(S_k)] - E[f(S_{k-1})] \geq \frac{1}{K} (f(O) - E[f(S_{k-1})]) - \delta.
\]
Therefore, by induction, we obtain
\[
E[f(S_K)] \geq \left(1 - \left(1 - \frac{1}{K}\right)^K\right) f(O) - \delta \sum_{k=0}^{K-1} \left(1 - \frac{1}{K}\right)^k \geq \left(1 - \frac{1}{e}\right) f(O) - \delta K,
\]
where we used \(f(\emptyset) = 0\). Hence we obtain the theorem from \(E[f(S)] = E[f(S_K)]\).

**Theorem 2.** If \((V, \mathcal{I})\) is a \(\kappa\)-extensible system with rank \(K\), we have \(E[f(S, \theta)] \geq \frac{1}{\kappa+1} f(O, \theta) - \delta K\).

**Proof.** For any realization of \(S_0 \subset S_1 \subset \cdots \subset S_K = S \in \mathcal{I}\), where \(K' \leq K\), we define \(S_{K'}, S_{K'+2}, \ldots, S_K \) as \(S_K\). We thus construct a series of feasible solutions, \(S_0, S_1, \ldots, S_K\), for any realization. Note that we have \(E[f(S)] = E[f(S_K)]\) since \(S = S_K\) for every realization.

We consider a series of random subsets \(O_0, \ldots, O_K\), where \(O_0 = O\). Our aim is to prove that we can construct such \(O_0, \ldots, O_K\) satisfying the following conditions: \(S_i \subseteq O_i \in \mathcal{I}\) (\(i = 0, \ldots, K-1\) and \(S_K = O_K \in \mathcal{I}\) for any realization, and
\[
\kappa \cdot (E[f(S_i)] - f(S_{i-1}) + \delta) \geq E[f(O_{i-1})] - E[f(O_i)] \quad (A1)
\]
for \(i = 1, \ldots, K\).

In the case of \(i = 0\), we have \(S_0 = \emptyset \subseteq O = O_0 \in \mathcal{I}\), and (A1) is not required to hold in this case.

We now assume that all random quantities are conditioned on an arbitrary realization of the \((k-1)\)-th step, where \(S_0, \ldots, S_{k-1}\) and \(O_0, \ldots, O_{k-1}\) satisfying \(S_i \subseteq O_i \in \mathcal{I}\) (\(i = 0, \ldots, k-1\)) are given. If \(S_{k-1}\) is maximal, we let \(O_k = S_k (= S_{k-1} = O_{k-1})\), which satisfies \(S_k = O_k \in \mathcal{I}\) and
\[
\kappa \cdot (E[f(S_k)] - f(S_{k-1}) + \delta) = \kappa \cdot \delta \geq 0 = f(O_{k-1}) - E[f(O_k)].
\]
If \(S_{k-1}\) is not maximal, from the definition of \(\kappa\)-extensible systems, for any choice of \(s_k \notin S_{k-1}\), there exists \(Z_k \subseteq O_{k-1} \setminus S_{k-1}\) such that \(O_{k-1} \setminus Z_k \cup \{s_k\} \in \mathcal{I}\) and \(|Z_k| \leq \kappa\) hold. We let \(O_k = O_{k-1} \setminus Z_k \cup \{s_k\}\). Note that thus constructed \(O_k\) satisfies \(S_k \subseteq O_k \in \mathcal{I}\) for any realization of the \(k\)-th step; moreover, if \(k = K\), we always have \(S_K = O_K \in \mathcal{I}\) since \(S_K\) is maximal in any realization. Considering expectation on the realization of the \(k\)-th step, we obtain
\[
\begin{align*}
&f(O_{k-1}) - E[f(O_k)] \\
&= f(O_{k-1}) - E[f(O_{k-1} \setminus Z_k)] \\
&\quad + E[f(O_{k-1} \setminus Z_k)] - E[f(O_k)] \\
&\leq E[f(O_{k-1} \setminus Z_k)] - E[f(O_k)] \quad \because O_{k-1} \setminus Z_k \subseteq O_k \text{ and monotonicity} \\
&\leq \sum_{v \in Z_k} f(s_{k-1}(v)) \quad \because S_{k-1} \subseteq O_{k-1} \setminus Z_k \text{ and submodularity} \\
&\leq \kappa \cdot (E[f(s_{k-1}(s_k))] + \delta) \quad \because S_{k-1} \cup Z_k \subseteq O_{k-1} \in \mathcal{I}, \text{ Lemma 1, and } |Z_k| \leq \kappa \\
&= \kappa \cdot (E[f(S_k)] - f(S_{k-1}) + \delta)
\end{align*}
\]
Therefore, in any case we have
\[
\kappa \cdot (E[f(S_k)] - f(S_{k-1}) + \delta) \geq f(O_{k-1}) - E[f(O_k)].
\]
By taking expectation on all realizations of the \((k-1)\)-th step, we obtain (A1) for \(i = k\). For every realization, \(O_0, \ldots, O_k\) constructed above satisfy \(S_i \subseteq O_i \in \mathcal{I}\) for \(i = 0, \ldots, k\); furthermore, if \(k = K\), \(S_K = O_K \in \mathcal{I}\) always holds. This means that the assumption of induction for the next step is satisfied. Consequently, (A1) holds for \(i = 1, \ldots, K\) by induction. Summing both sides of (A1) for \(i = 1, \ldots, K\), we obtain
\[
\kappa \cdot (E[f(S_K)] - f(\emptyset) + \delta K) \geq E[f(O_0)] - E[f(O_K)].
\]
Since we always have \(f(\emptyset) = 0, O_0 = O, \text{ and } O_K = S_K\) for any realization, it holds that
\[
E[f(S_K)] \geq \frac{1}{\kappa + 1} f(O) - \frac{\kappa}{\kappa + 1} \delta K \geq \frac{1}{\kappa + 1} f(O) - \delta K.
\]
Hence we obtain the theorem from \(E[f(S)] = E[f(S_K)]\). \(\square\)
C Regularization functions

We first detail the case where the regularization function is given by the entropy function. We then discuss how to design regularization functions that satisfy Assumption 2.

C.1 Entropy function

We consider using the following entropy function as a regularization function:

$$\Omega_k(p) = \epsilon \sum_{u \in U_k} p(u) \ln p(u),$$

where $\epsilon > 0$ is a constant that controls the perturbation strength. Note that we have $\Omega_k(p) - \Omega_k(q) \leq \epsilon \cdot 0 - \epsilon \sum_{i=1}^{n_k} \frac{1}{n_k} \ln \frac{1}{n_k} = \epsilon \ln n_k$ for any $p, q \in \Delta^{n_k}$.

In this case, from the relationship between the entropy regularization and softmax, each iteration of SMOOTHED GREEDY can be performed via softmax sampling. More precisely, from the Karush–Kuhn–Tucker (KKT) condition of problem (2), $\max_{p \in \Delta^{n_k}} \{ \langle g_k, p \rangle - \Omega_k(p) \}$, we have

$$\epsilon (\ln p + 1_{n_k}) - g_k + 1_{n_k} \mu = 0_{n_k} \quad \text{and} \quad 1_{n_k}^T p = 1, \quad (A2)$$

where $\ln \cdot$ operates in an element-wise manner and $\mu \in \mathbb{R}$ is a multiplier corresponding to the equality constraint. Note that we need not take the inequality constraints, $p \geq 0_{n_k}$, into account since the entropy regularization forces every $p(u)$ to be positive. Since $\Omega_k$ is strictly convex and every feasible solution satisfies the linear independence constraint qualification (LICQ), the maximizer, $p_k$, is characterized as the unique solution to the KKT equation system (A2). From (A2), we see that $p_k$ is proportional to $\exp(g_k)/\epsilon$. Hence Steps 4–6 of Algorithm 1 can be substituted via softmax sampling: $p_k(u, \theta) \propto \exp(f_{S_k-1}(u, \theta)/\epsilon)$ for $u \in U_k$.

We then consider computing $\nabla_{g_k} p_k(g_k)$. While this can be done by directly differentiating $p_k(u, g_k) \propto \exp(g_k(u)/\epsilon)$, we here see how to obtain it by applying the implicit function theorem (see, e.g., [13]) to the KKT equation system (A2) as a warm-up for the next section. In this case, the requirements for using the implicit function theorem are satisfied (see the next section). By differentiating the KKT equation system (A2) w.r.t. $g_k$, we obtain

$$\left[ \epsilon \text{diag}(p_k)^{-1} \right] \begin{bmatrix} 1_{n_k} \\ 0 \end{bmatrix} \begin{bmatrix} \nabla_{g_k} p_k \\ \nabla_{g_k} \mu \end{bmatrix} = \begin{bmatrix} 0_{n_k} \\ 1_{n_k} \end{bmatrix},$$

where $\text{diag}(p_k)$ is a diagonal matrix whose diagonal entries are $p_k$ and $1_{n_k}$ is the $n_k \times n_k$ identity matrix. We can compute $\nabla_{g_k} p_k$ by solving the above equation as follows:

$$\begin{bmatrix} \nabla_{g_k} p_k \\ \nabla_{g_k} \mu \end{bmatrix} = \left[ \epsilon \text{diag}(p_k)^{-1} \right] \begin{bmatrix} 1_{n_k} \\ 0 \end{bmatrix}^{-1} \begin{bmatrix} 0_{n_k} \\ 1_{n_k} \end{bmatrix} = \left[ \epsilon^{-1}(\text{diag}(p_k) - p_k p_k^T) \right] p_k.$$

C.2 Regularization functions satisfying Assumption 2

For any differentiable $\Omega_k$, the KKT condition of problem (2) can be written as

$$\nabla_p \Omega_k(p) - g_k - \lambda + 1_{n_k} \mu = 0_{n_k}, \quad \lambda \odot p = 0_{n_k}, \quad \text{and} \quad 1_{n_k}^T p = 1,$$

where $\lambda \geq 0_{n_k}$ consists of multipliers corresponding to the inequality constraints and $\odot$ denotes the element-wise product. Since every feasible point in $\Delta^{n_k}$ satisfies LICQ, if $\Omega_k$ is strictly convex on $\Delta^{n_k}$, the optimal solution is uniquely characterized by the KKT condition. Let $(\hat{p}, \lambda, \mu)$ be a triplet satisfying the KKT condition, where $\hat{p} = p_k$. If $\Omega_k$ is twice-differentiable, the Hessian $\nabla^2_p \Omega_k(\hat{p})$, is positive definite, and the strict complementarity, $\lambda + \hat{p} > 0_{n_k}$, holds, then $\nabla_{g_k} p_k$ can be calculated from the KKT condition as detailed below (see, also [3]). Summarizing the above, a sufficient condition for satisfying Assumption 2 can be written as follows:

1. $\Omega_k$ is twice-differentiable,
2. $\nabla^2_p \Omega_k(p)$ is positive definite for any $p \in \Delta^{n_k}$ (this implies the strict convexity), and
3. the strict complementarity holds at the unique optimum, $p_k$. 

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In practice, given any twice-differentiable convex function, we can add to it the entropy function multiplied by a small constant for obtaining $\Omega_k$ that satisfies the above sufficient condition.

We explain how to compute $\nabla g_k p_k$. Let $\bar{U}$ be a subset of $U_k$ such that $\bar{p}(u) = 0$ iff $u \in \bar{U}$; the strict complementarity implies $\bar{\lambda}(u) = 0$ iff $u \notin \bar{U}$. We let $x := (p, \lambda, \mu)$, where $\lambda \in R^{|U|}$-dimensional vector consisting of entries of $\lambda$ corresponding to $\bar{U}$. We define $I_\bar{U}$ as a $n_k \times |U|$ matrix that has columns of $I_{n_k}$ corresponding to $\bar{U}$. The KKT equation system can be rewritten as

$$H(x, g_k) := \left[ \begin{array}{c} \nabla p \Omega_k(p) - g_k - I_\bar{U} \lambda + 1_{n_k} \mu \\ -I_\bar{U}^\top p \\ 1_{n_k}^\top p - 1 \end{array} \right] = \left[ \begin{array}{c} 0_{n_k} \\ 0_{|U|} \\ 0 \end{array} \right].$$

at $\bar{x} = (\bar{p}, \bar{\lambda}, \bar{\mu})$, and its partial Jacobians at $\bar{x}$ are

$$\nabla_x H(\bar{x}, g_k) = \left[ \begin{array}{c} \nabla^2 \Omega_k(\bar{p}) & -I_\bar{U} & 1_{n_k} \\ -I_\bar{U}^\top & 0_{|U|+1 \times |U|+1} \end{array} \right]$$

and

$$\nabla g_k H(\bar{x}, g_k) = \left[ \begin{array}{c} -1_{n_k} \\ 0_{|U| \times n_k} \\ 0_{n_k} \end{array} \right].$$

Note that $|\bar{U}| < n_k$ always holds; otherwise $\bar{p} = 0_{n_k}$, which is an infeasible solution. Therefore, $[-I_\bar{U} 1_{n_k}]$ always has rank $|\bar{U}| + 1$. From the positive definiteness of $\nabla^2 \Omega_k(\bar{p})$, we have

$$\det(\nabla_x H(\bar{x}, g_k)) = \det(\nabla^2 \Omega_k(\bar{p})) \det((-[-I_\bar{U} 1_{n_k}]^\top \nabla^2 \Omega_k(\bar{p})^{-1}[-I_\bar{U} 1_{n_k}]) \neq 0,$$

where we used the Schur complement; hence $\nabla_x H(\bar{x}, g_k)$ is non-singular. This guarantees that $\nabla g_k p_k$ can be computed by using the implicit function theorem as follows:

$$\left[ \begin{array}{c} \nabla g_k p_k \\ \nabla g_k \lambda_\bar{U} \\ \nabla g_k \mu \end{array} \right] = -\nabla_x H(\bar{x}, g_k)^{-1} \nabla g_k H(\bar{x}, g_k).$$

A recent result by Stechlinski et al. [47] provides an extended version of the implicit function theorem, which may enable us to deal with a wider class of $\Omega_k$; we leave discussion on this for future work.

D Discussion on other gradient estimators

The score-function gradient estimator is one of major Monte Carlo gradient estimators. Other than that, the pathwise and measure-valued gradient estimators are widely used (see, [36] for a survey). We discuss why it is difficult to apply these methods to our case. The pathwise gradient estimators basically use derivatives of quantities inside the expectation. In our case, however, it is impossible to differentiate the quantity, $Q(S)$, w.r.t. $S$. When computing the measure-valued gradient estimators, we decompose $\nabla \theta p(\theta)$ into $p^+(\theta)$ and $p^-(\theta)$ so that both $p^+(\theta)$ and $p^-(\theta)$ form some probability distribution functions, where $\nabla \theta p(\theta) = c_\theta (p^+(\theta) - p^-(\theta))$ must hold with some constant $c_\theta$. Then, we can estimate the gradient by sampling from $p^+(\theta)$ and $p^-(\theta)$. Such a decomposition is possible when $p(\theta)$ has well-known structures, e.g., Poisson and Gaussian. However, if $p(\theta)$ is the output distribution, how to decompose $p(\theta)$ is non-trivial and seems to be very complicated.

E Learning submodular models with oracle queries

We discuss application of our framework to learning of parameterized submodular functions, and we provide experimental results.

E.1 Problem description

We consider maximizing unknown submodular function $\hat{f}(\cdot)$ by sequentially querying its values. Specifically, in each $t$-th round, we can query $\hat{f}(\cdot)$ values at $N$ points $s_1, \ldots, s_N \in \mathcal{I}$, and, by using this feedback, we aim to find a good solution for maximizing $\hat{f}(\cdot)$. We assume that no prior knowledge on $\hat{f}(\cdot)$ is available and that to query the true function value is time consuming. We aim to achieve high $\hat{f}(\cdot)$ values with a small number of rounds and queries. One can think of this setting
as a variant of submodular maximization with low adaptive complexities [5] and online submodular maximization with bandit feedback [56]. We here consider the following approach: we construct some parameterized submodular model \( f(\cdot, \theta) \), e.g., a deep submodular function, and update \( \theta \) by using our gradient estimators with \( Q(S_j) = \hat{f}(S_j) \). Namely, akin to the decision-focused method explained in Section 4.1, we train \( f(\cdot, \theta) \) so that the greedy algorithm can achieve high \( \hat{f}(\cdot) \) values; the current setting is more difficult since we know nothing about \( \hat{f}(\cdot) \) in advance and features, which are used by the predictive models, are unavailable.

E.2 Experiments

We use the corporate leadership network dataset of KONECT [32], which contains person–company leadership information between 20 people and 24 companies; the companies are indexed with \( i = 1, \ldots, 24 \). We let each \( v \in V \) represent a person, who is associated with a subset of companies \( I_v \subseteq \{1, \ldots, 24\} \). We define \( I_X := \bigcup_{v \in X} I_v \) for every \( X \subseteq V \). We express the importance of the \( i \)-th company with a non-negative weight \( w_i \); we here let \( w_1 = w_3 = \cdots = w_{23} = 1 \) and \( w_2 = w_4 = \cdots = w_{24} = 0.1 \). We use the weighted coverage function as an unknown true function: \( \hat{f}(X) := \sum_{i \in I_X} w_i \). We separate the 20 people into two groups of 10 people, and we consider choosing up to two people from each group; i.e., \((V, I)\) forms a partition matroid.

As a model function, \( f(\cdot, \theta) \), we use a deep submodular function that forms a 2-layer NN. We set the hidden-layer size at 50 and use sigmoid activation functions. We set initial NN parameters \( \theta \) at random non-negative values drawn from \([0, 0.01]\).
For $t = 1, \ldots, 20$, we perform SMOOTHED GREEDY $N$ times with objective function $f(\cdot, \theta)$ to obtain $S_1, \ldots, S_N$. We then query $\hat{f}(S_1), \ldots, \hat{f}(S_N)$ values to compute the gradient estimator, and we update $\theta$ by using Adam with learning rate $10^{-3}$. We also consider a noisy setting where observed $\hat{f}(S_j)$ values are perturbed with random variables drawn from the standard normal distribution. We here use the entropy function with $\epsilon = 0.02$ as a regularization function of SMOOTHED GREEDY.

As in Section 5.2, (VR-)SG-$N$ stands for (variance-reduced) SMOOTHED GREEDY with $N$ samples. In each $t$-th round, we evaluate trained $f(\cdot, \theta)$ as follows: we obtain $S \in \mathcal{I}$ by applying the greedy algorithm to $\hat{f}(\cdot, \theta)$, and we compute model function value $f(S, \theta)$ and true function value $\hat{f}(S)$. **Oracle-Greedy** is the greedy algorithm directly applied to $\hat{f}(\cdot)$, which we cannot do in practice. **Random** returns $X \in \mathcal{I}$ by randomly choosing two people from each of the two groups.

Figure 2 presents the means and standard deviations of model and true function values calculated over 30 random trials. We see that we can improve true function values by updating and maximizing the model function. As indicated by the results of SG-$1$, if even once we can query $\hat{f}(\cdot)$ value in each round, we can do better than Random. With more queries and the variance reduction method, we achieve higher true function values. The results suggest that our method is effective for learning and maximizing submodular functions when only a limited amount of feedback is available.