Abstract

Motivated by an application to $\ell_0$-constrained minimization, the maximization of set functions with weak submodularity and weak supermodularity, which we call weakly modular functions, has recently become an interesting research topic. In this paper, we make theoretical and practical contributions to this topic. On the theoretical side, we prove that it is hard to improve an existing approximation guarantee, and we also show that the problem is fixed-parameter-tractable under certain conditions. On the practical side, we prove guarantees of efficient multi-stage algorithms and confirm their advantages via experiments.

1 Introduction

We consider the following maximization problem:

$$\maximize_{S \subseteq [d]} F(S) \text{ subject to } |S| \leq k,$$

where $[d] := \{1, \ldots, d\}$ and $F : 2^{[d]} \to \mathbb{R}$ is a monotone set function that has weak submodularity and weak supermodularity (or bounded submodularity and supermodularity ratios), which we call a weakly modular function. As illustrated in Figure 1 weakly modular functions form a class that is close to modular functions, and so we expect the class to have some nice properties. A major application of weakly modular maximization (1) is the following $\ell_0$-constrained minimization, an important problem in machine learning:

$$\minimize_{x \in \mathbb{R}^d} l(x) \text{ subject to } \|x\|_0 \leq k,$$

where $l : \mathbb{R}^d \to \mathbb{R}$ is a differentiable objective function and $\|x\|_0$ is the number of non-zeros of $x$; the resulting feasible region is non-convex. We assume that $l(\cdot)$ has restricted strong convexity (RSC) and restricted smoothness (RSM) as detailed later; this assumption is common in many previous studies [20, 39]. Recent studies [12, 5] have revealed that, if $l(\cdot)$ has RSC and RSM, then the following set function $F$ is weakly modular:

$$F(S) := l(0) - \min_{\text{supp}(x) \subseteq S} l(x).$$

Thanks to this fact, we can address problem (2) leveraging various set-function maximization techniques, and so weakly modular maximization has been becoming a promising approach. The importance of weakly modular maximization is also supported by many other applications [3, 5]. However, since it is an emerging topic and the connection to RSC/RSM has been revealed very recently, few studies have yet been undertaken.

A well-known result is a $(1 - e^{-\gamma_{S,k}}$)-approximation guarantee of the greedy algorithm (Greedy) for weakly submodular maximization [14], where $S \subseteq [d]$ is the solution of Greedy and $\gamma_{S,k} \in [0, 1]$ is the submodularity ratio of $F$, which we detail later. However, other than this, we have little theoretical insight into problem (1). In particular, the following questions are still open: Can we improve the $(1 - e^{-\gamma_{S,k}}$)-approximation guarantee by using a bounded supermodularity ratio, and how costly would it be to solve the problem (almost) optimally?

When it comes to practical algorithms, projected-gradient-based methods for problem (2) (e.g., iterative hard thresholding (IHT) [4] and hard thresholding pursuit (HTP) [15]) have been extensively studied thanks to their efficiency. Compared to them, greedy-style methods, such as Greedy (or forward greedy selection) and orthogonal

\footnote{There are several variations of forward greedy selection, and we call the one presented in [12] Greedy in the context of $\ell_0$-constrained minimization.}
matching pursuit (OMP) [30], are often slow. Regarding theoretical guarantees, however, greedy-style methods tend to be more resistant to the ill condition than IHT/HTP, and this is empirically true as we will see via experiments. Therefore, it is desirable to develop greedy-style methods that can run as fast as IHT/HTP and perform well with ill-conditioned instances.

1.1 Our Contribution

As posed above, weakly modular maximization has several problems awaiting solutions both in theory and practice. We address such problems and make three contributions as detailed below. All proofs are provided in the appendix.

Hardness. In Section 3 we prove that the \((1 - e^{-\gamma S, k})\)-approximation guarantee of Greedy is optimal for a certain class of weakly modular maximization. We first explain that an existing improved guarantee [3] that uses curvature cannot be used in our case. We then prove that no polynomial-time algorithms can improve the \((1 - e^{-\gamma S, k})\)-approximation guarantee in the value oracle model for a class of weakly modular maximization where submodularity and supermodularity ratios defined on certain subsets are bounded. Although the class of problems being considered is limited, this is the first hardness result related to improving the approximation factor for non-submodular maximization. Our result also suggests that it is hardly possible to obtain a better guarantee for easier classes of weakly modular maximization simply by modifying the proof of Greedy.

Fixed-parameter tractability. In Section 4 we study how costly it is to solve weakly modular maximization almost optimally. Specifically, based on the idea of [34], we develop a randomized fixed-parameter-tractable (FPT) approximation algorithm (Rand-FPT-Approx) for problem (1), which can compute arbitrarily good solutions at the expense of FPT computation time. As a corollary of this result, we show that \(\epsilon\)-error solutions for \(\ell_0\)-constrained minimization can be computed at the cost of FPT time. Most existing guarantees for \(\ell_0\)-constrained minimization [33, 20] require that sparsity \(k\) is sufficiently large. In contrast, our result holds without requiring such a condition for \(k\). Instead, we have a trade-off between the computation cost and error magnitude \(\epsilon\). This kind of trade-off for \(\ell_0\)-constrained minimization has not been proved elsewhere to the best of our knowledge.

Multi-stage algorithms. In Section 5 we consider using the multi-stage approach [26, 38] to speed up greedy-style methods. With this approach, instead of choosing one element, we choose multiple elements in each iteration, thus reducing the running time. While this approach yields accelerated greedy-style algorithms, how to prove their performance guarantees for weakly modular maximization and \(\ell_0\)-constrained minimization is non-trivial. We first prove a guarantee of the multi-stage greedy algorithm (Multi-Greedy) for weakly modular maximization. This result includes the existing \((1 - e^{-\gamma S, k})\)-approximation guarantee of Greedy [10] as a special case. We also present a guarantee of Multi-Greedy for \(\ell_0\)-constrained minimization by using the connection between RSC/RSM and weak modularity. We then focus on \(\ell_0\)-constrained minimization and prove a guarantee of the multi-stage OMP (Multi-OMP). Somewhat surprisingly, this result matches that of the standard OMP shown in [12]. Experiments show that the multi-stage algorithms can outperform IHT/HTP both in terms of running time and solution quality, particularly when the instances are ill-conditioned as is expected.

1.2 Related Work

Monotone submodular maximization of form (1) has been widely studied. Nemhauser et al. [29] proved the \((1 - e^{-1})\)-approximation guarantee of Greedy, and it is hard to improve the guarantee in polynomial time; more precisely, Nemhauser & Wolsey [28] proved the hardness in the value oracle model, and Feige [13] proved the NP-hardness for Max \(k\)-cover. Our hardness result can be seen as a weakly modular version of the former result. Skowron [34] developed a randomized FPT approximation algorithm for a subclass of monotone submodular maximization. We
extend this result to weakly modular maximization. Wei et al. studied multi-stage algorithms for the monotone submodular maximization, but no guarantees have been proved for maximization of non-submodular functions, including weakly modular functions.

When it comes to non-submodular maximization, various notions have been introduced to obtain theoretical guarantees. One of the most prevalent is the submodularity ratio, which has been used in many studies. The curvature, another notion that appears in many studies, is defined by (3). We will show that weak supermodularity can also be derived from RSC/RSM. These two results imply that, if \( l(\cdot) \) is well-conditioned in terms of RSC/RSM, \( F(\cdot) \) is close to a modular function.

Liberty & Sviridenko studied weakly supermodular minimization; however, we can see that their definition of weak supermodularity is close to that of weak submodularity by considering the negative of the objective function. Their results that use the supermodularity ratio are different from existing guarantees that use the curvature. Unlike their result, our hardness result considers every polynomial-time algorithm in the value oracle model.

2 Preliminaries

Below we introduce the notation and definitions that we employ, and then we show the connection between RSC/RSM and weak supermodularity.

\[ 2.1 \text{ Notation and Definitions} \]

**Sets and set functions.** We denote subsets of \([d]\) with upper case sans-script fonts: e.g., \(S\) and \(T\). Elements in \([d]\) are basically denoted by \(j\). We sometimes abuse the notation and denote \(\{j\} \subseteq [d]\) simply by \(j\). We use upper case letters (e.g., \(F\) and \(G\)) for set functions on \(2^d\). Given any set function \(F\), we let \(F(T | S) := F(S \cup T) - F(S)\) for any \(S, T \subseteq [d]\). All the set functions considered in this paper are monotone (i.e., \(F(T | S) \geq 0\) for any \(S, T \subseteq [d]\)) and normalized (i.e., \(F(\emptyset) = 0\)). We say \(F\) is submodular (supermodular) if it satisfies \(F(j | S) \geq F(j | T)\) for any \(S \subseteq T\) and \(j \notin T\). Throughout this paper, we assume that \(F(\cdot)\) can be evaluated efficiently. In particular, in Section 2.1 we assume it can be evaluated in polynomial time w.r.t. \(d\) (or poly(d) time).

If \(F(\cdot)\) is defined by (3), we can compute \(F(S)\) by solving \(\min_{\supp(x) \subseteq S} l(x)\). Given a quadratic \(l(\cdot)\), we can solve it by computing a pseudo-inverse matrix. Given a more general \(l(\cdot)\), we can use iterative methods (e.g., (32)) to solve the minimization problem.

**Submodularity and supermodularity ratios.** Given monotone \(F : 2^d \to \mathbb{R}\), its weak submodularity and weak supermodularity are parametrized with the following submodularity and supermodularity ratios, respectively. Let \(U \subseteq [d]\) and \(k \geq 1\) be a fixed subset and an integer, respectively. We define the submodularity ratio \(\gamma_{U,k}\) and supermodularity ratio \(\tilde{\gamma}_{U,k}\) of \(F(\cdot)\) as the largest scalars that satisfy

\[
\gamma_{U,k} F(S | L) \leq \sum_{j \in S} F(j | L) \leq \tilde{\gamma}_{U,k} F(S | L)
\]

for any disjoint \(L, S \subseteq [d]\) such that \(L \subseteq U\) and \(|S| \leq k\). Note that we have \(\gamma_{U,k} \leq \gamma_{U',k'}\) and \(\tilde{\gamma}_{U,k} \leq \tilde{\gamma}_{U',k'}\) for any \(U' \subseteq U\) and \(k' \leq k\). We can confirm that \(\gamma_{U,k} \in [0,1]\) and \(\tilde{\gamma}_{U,k} \in [1/k, 1]\) hold for any \(U\) and \(k\). We define
\( \gamma_{k', k} := \min_{|l| \leq k'} \gamma_{k, k} \) and \( \tilde{\gamma}_{k', k} := \min_{|l| \leq k'} \tilde{\gamma}_{k, k} \). We have \( \gamma_{d, d} = 1 \) and \( \tilde{\gamma}_{d, d} = 1 \) iff \( F(\cdot) \) is submodular (supermodular). We say \( F \) is \( (\gamma_{U, k}, \tilde{\gamma}_{U, k}) \)-weakly modular if \( F \) has the submodularity ratio \( \gamma_{U, k} \) and supermodularity ratio \( \tilde{\gamma}_{U, k} \).

Curvature and inverse curvature. Given monotone \( F : 2^{|d|} \rightarrow \mathbb{R} \), its curvature \( \alpha \in [0, 1] \) and inverse curvature \( \tilde{\alpha} \in [0, 1] \) are defined as the smallest scalars that satisfy

\[
F(j \mid S \setminus \{j\} \cup M) \geq (1 - \alpha)F(j \mid S \setminus \{j\}),
\]

\[
F(j \mid S \setminus \{j\}) \geq (1 - \tilde{\alpha})F(j \mid S \setminus \{j\} \cup M),
\]

respectively, for any \( S, M \subseteq [d] \) and \( j \in S \setminus M \). Function \( F \) is submodular (supermodular) iff \( \tilde{\alpha} = 0 \) (\( \alpha = 0 \)).

Vectors and matrices. Bold lower case letters (e.g., \( x \) and \( y \)) denote vectors, and zero vectors are denoted simply by 0. Given \( S \subseteq [d] \) and \( x \in \mathbb{R}^{|d|} \), whose \( j \)-th entry is associated with \( j \in [d] \), \( x_S \in \mathbb{R}^S \) denotes the restriction of \( x \) to \( S \). Lower case letters (e.g., \( l \) and \( f \)) denote functions on \( \mathbb{R}^{|d|} \). Bold upper case letters (e.g., \( A \) and \( B \)) denote matrices.

Restricted strong convexity and restricted smoothness. Let \( l : \mathbb{R}^{|d|} \rightarrow \mathbb{R} \) be a differentiable function. Given \( \Omega \subseteq \mathbb{R}^{|d|} \times \mathbb{R}^{|d|} \), we say \( l(\cdot) \) is \( \mu_{\Omega} \)-RSC and \( \nu_{\Omega} \)-RSM if it satisfies

\[
\frac{\mu_{\Omega}}{2} \|y - x\|^2 \leq l(y) - l(x) - \langle \nabla l(x), y - x \rangle \leq \frac{\nu_{\Omega}}{2} \|y - x\|^2
\]

for all \( (x, y) \in \Omega \). We refer to \( \mu_{\Omega} \) and \( \nu_{\Omega} \) as RSC and RSM constants, respectively. If \( l(\cdot) \) is quadratic, then the above inequality of RSC/RSM reduces to that of the well-known restricted isometric property (RIP) condition [6]. Note that, given \( \mu_{\Omega} \) and \( \nu_{\Omega} \), and \( \Omega' \subseteq \Omega \), we can set \( \mu_{\Omega'} \geq \mu_{\Omega} \) and \( \nu_{\Omega'} \leq \nu_{\Omega} \), respectively. If \( l(\cdot) \) is \( \mu_{\Omega} \)-RSC and \( \nu_{\Omega} \)-RSM with \( \Omega' = \{(x, y) \in \mathbb{R}^{|d|} \times \mathbb{R}^{|d|} \mid \|x\| \leq k_1, \|y\| \leq k_1, \|x - y\| \leq k_2 \} \), we say \( l(\cdot) \) is \( \mu_{k_1, k_2} \)-RSC and \( \nu_{k_1, k_2} \)-RSM. We define \( \mu_k := \mu_{k, k} \) and \( \nu_k := \nu_{k, k} \). If \( l(\cdot) \) is \( \mu_{\Omega} \)-RSC and \( \nu_{\Omega} \)-RSM with \( \Omega = \mathbb{R}^{|d|} \times \mathbb{R}^{|d|} \), we abbreviate \( \Omega \) and say \( l(\cdot) \) is \( \mu \)-strongly convex (\( \mu \)-SC) and \( \nu \)-smooth (\( \nu \)-SM).

2.2 RSC and RSM Imply Weak Modularity

We assume that \( F(\cdot) \) is defined by \( [3] \). Ellenberg et al. [12] showed that the submodularity ratio \( \gamma_{U, k} \) of \( F(\cdot) \) can be bounded from below with RSC and RSM constants of \( l(\cdot) \). Furthermore, Bogunovic et al. [5] showed that the supermodularity ratio \( \tilde{\gamma}_{U, k} \) of \( F(\cdot) \) is bounded with SC and SM constants. By using these results and slightly extending the later one, we can show that \( F(\cdot) \) is a weakly modular function whose ratios are bounded with RSC and RSM constants. The following lemma is a key to proving this result.

Lemma 1 (implied in [12]). For any \( A \subseteq [d] \), let \( b^{(A)} := \arg\min_{\text{supp}(x) \subseteq A} l(x) \). For any disjoint \( A, B \subseteq [d] \), if \( l(\cdot) \) is \( \mu_{|A|, |B|} \)-RSC and \( \nu_{|A|, |B|} \)-RSM, we have

\[
\frac{\|\nabla l(b^{(A)})_B\|_2^2}{2\nu_{|A|, |B|}} \leq F(B \mid A) \leq \frac{\|\nabla l(b^{(A)})_B\|_2^2}{2\mu_{|A|, |B|}}.
\]

Intuitively, the lemma connects the decrease in \( l(\cdot) \) to the increase in \( F(\cdot) \). Actually, we can slightly strengthen the lemma (see, the appendix), but we here present the weaker version for convenience. By using this lemma, we obtain the following proposition:

Proposition 1 (partially adopted from [12] [5]). For any \( U \subseteq [d] \) and \( k \in \mathbb{Z}_{>0} \), the submodularity ratio \( \gamma_{U, k} \) and supermodularity ratio \( \tilde{\gamma}_{U, k} \) of \( F(\cdot) \) are bounded with RSC and RSM constants of \( l(\cdot) \) as

\[
\gamma_{U, k} \geq \frac{\mu_{|U| + k}}{\nu_{|U| + 1, 1}} \geq \frac{\mu_{|U| + k}}{\nu_{|U| + k}} =: \frac{1}{\kappa_{|U| + k}},
\]

\[
\tilde{\gamma}_{U, k} \geq \frac{\mu_{|U| + 1}}{\nu_{|U| + k, k}} \geq \frac{\mu_{|U| + k}}{\nu_{|U| + k}} =: \frac{1}{\kappa_{|U| + k}}.
\]

We call \( \kappa_{|U| + k} := \nu_{|U|} / \mu_{|U| + 1} \geq 1 \) a restricted condition number [19]; problem [2] with a smaller \( \kappa_{|U| + k} \) is typically easier to deal with. On the other hand, from the definitions of \( \gamma_{U, k} \) and \( \tilde{\gamma}_{U, k} \), we have \( F(S \mid L) \approx \sum_{j \in S} F(j \mid L) \) if \( \kappa_{|U| + k} \approx 1 \). Namely, a small \( \kappa_{|U| + k} \) implies that \( F(\cdot) \) is close to a modular function.
3 Hardness Result

For weakly submodular maximization, Das & Kempe [10] proved that Greedy can find a solution $S \subseteq [d]$ that is guaranteed to achieve a $(1 - e^{-75\cdot k})$-approximation. When it comes to weakly modular maximization, both the submodularity ratio and the supermodularity ratio are bounded. Therefore, we can expect a better guarantee to be possible by using the bounded supermodularity ratio. Bian et al. [3] addressed a similar research topic and proved that, if $F$ has the submodularity ratio $\gamma_{S,k}$ and curvature $\alpha$, Greedy is guaranteed to achieve a $\frac{\alpha}{\gamma_{S,k}}(1 - e^{-\alpha\gamma_{S,k}})$-approximation. Below we first elucidate the relationship between the curvature and supermodularity ratio; in short, even if the supermodularity ratio is bounded, curvature $\alpha$ can be unbounded (i.e., $\alpha = 1$). Hence the $\frac{\alpha}{\gamma_{S,k}}(1 - e^{-\alpha\gamma_{S,k}})$-approximation guarantee does not help us to obtain a better guarantee for weakly modular maximization in general. We then prove the following hardness result. Even if the supermodularity ratio $\tilde{\gamma}_{k,k}$ is bounded by a constant smaller than $1/2$, no algorithms that evaluate $F$ only polynomially many times can achieve an approximation guarantee that exceeds $1 - e^{-75\cdot k}$ in general.

3.1 Ratios and Curvatures

Bogunovic et al. [5] proved the following relationship between ratios, $\gamma_{U,k}, \tilde{\gamma}_{U,k}$, and curvatures, $\alpha, \tilde{\alpha}$:

**Proposition 2** (Bogunovic et al. [5]). For any $U \subseteq [d]$ and $k \in \mathbb{Z}_{>0}$, we have

$$\gamma_{U,k} \geq 1 - \tilde{\alpha} \quad \text{and} \quad \tilde{\gamma}_{U,k} \geq 1 - \alpha.$$  

Therefore, weakly submodular functions with bounded curvatures, which were studied by Bian et al. [3], can be seen as weakly modular functions. Although a bounded curvature implies a bounded supermodularity ratio, the opposite is not always true. In fact, there exists an $\ell_{0}$-constrained minimization instance such that $F(\cdot)$ of form (3) has unbounded curvatures and bounded ratios (see, the appendix for details).

**Proposition 3.** There exists an instance of form (2) that satisfies the following conditions: $F(\cdot)$ defined as in (3) has curvatures $\alpha = \tilde{\alpha} = 1$, and $l(\cdot)$ that defines $F(\cdot)$ has condition number $\kappa := \nu/\mu \geq \frac{3 + \sqrt{5}}{3 - \sqrt{5}}$, which means $F(\cdot)$ has $\gamma_{U,k} \geq \frac{3 - \sqrt{5}}{3 + \sqrt{5}}$ and $\tilde{\gamma}_{U,k} \geq \frac{3 - \sqrt{5}}{3 + \sqrt{5}}$ for any $U$ and $k$.

Therefore, when considering application to $\ell_{0}$-constrained minimization, the curvature-dependent approximation factor, $\frac{1}{\kappa}(1 - e^{-\alpha \gamma_{U,k}})$, does not help us to improve the $1 - e^{-75\cdot k}$ approximation guarantee. We remark that a better guarantee can possibly be obtained by using greedy curvature $\alpha^G \leq \alpha$ [3]. However, to the best of our knowledge, no upper bound of $\alpha^G$ has been proved for $F(\cdot)$ defined as in (3). Taking these facts into account, the following question naturally arises: Can we improve the $(1 - e^{75\cdot k})$-approximation guarantee by using a bounded supermodularity ratio? Below we present a hardness result that partially answers this question.

3.2 Main Theorem

Our hardness result is as follows:

**Theorem 1.** Consider a class of weakly modular maximization satisfying the following conditions: $F$ is monotone and has a submodularity ratio $\gamma_{k,k} = 1$ and a supermodularity ratio $\tilde{\gamma}_{k,k} \geq 1/2 - o(1)$. For this class, no algorithms that evaluate $F$ only on polynomially many subsets can achieve an approximation guarantee that exceeds $1 - e^{-1} = 1 - e^{-\gamma_{k,k}}$.

Given solution $S$ of Greedy, we have $\gamma_{S,k} \geq \gamma_{k,k}$. Hence Theorem 1 implies the following fact. Even if $\gamma_{k,k} \leq \gamma_{S,k}$ is lower bounded by a constant that can be arbitrarily close to $1/2$, no polynomial-time algorithms can improve the $(1 - e^{-75\cdot k})$-approximation guarantee of Greedy in the value oracle model in general. We emphasize that the considered class is different from the standard monotone submodular maximization in that $\gamma_{k,k}$ is bounded by a constant, which means our result does not reduces to the existing result [23]. Theorem 1, however, does not hold for some easier classes of weakly modular maximization. Below we present a discussion of this issue.

**Discussion.** For example, the following easier class is not considered in Theorem 1. The ratios defined on the whole domain (i.e., $\gamma_{d,d}$ and $\tilde{\gamma}_{d,d}$) are bounded by constants. Therefore, with regard to algorithms whose guarantees are proved by using (weak) submodularity over the whole domain, their guarantees may be improved by using bounded $\gamma_{d,d}$. One such algorithm is the continuous greedy algorithm [37], and so a better guarantee of weakly modular maximization may be possible by using continuous-greedy-based methods. However, whether this approach works or not is non-trivial since we are currently missing a guaranteed rounding scheme for weakly modular functions. On the other hand, as in [10, 3], the proofs of Greedy rely only on weak submodularity defined on the restricted domain (or bounded $\gamma_{k,k}$). With regard to such algorithms, Theorem 1 suggests that, even if $\gamma_{d,d}$ and $\tilde{\gamma}_{d,d}$ are bounded, it is
Suppose that

\[ x^* = \arg\min_{x} \{ F(x) | S_{i-1} \}. \]

The detail of the algorithm is shown in Algorithm 1, which performs

\[ \ell_0 \]-constrained minimization. The problem is NP-hard in general [27], and so it is almost impossible to guarantee that polynomial-time algorithms such as Greedy and IHT can always find optimal solutions. Furthermore, the guarantees of such polynomial-time algorithms often require that a sufficient number of entries are allowed to be non-zero. For example, the guarantee of Greedy can be written as follows:

**Proposition 4** (Elenberg et al. [12]). Let \( x^* \) be an optimal solution for problem (2), \( S^* := \text{supp}(x^*) \), and \( k^* := |S^*| \). Suppose that \( F \) is defined as in (3), where \( l(\cdot) \) is assumed to have a restricted condition number \( \kappa_{k+k^*} \). Let \( S \) be an output of Greedy. Then \( F(S) \geq (1 - \exp(-\frac{1}{\kappa_{k+k^*}}))F(S^*) \) holds. Consequently, if we have

\[ k \geq k^* \times \kappa_{k+k^*}, \log \left( \frac{l(0) - l(x^*)}{\epsilon} \right), \]

\( x = \arg\min_{\text{supp}(x') \subseteq S} l(x') \) satisfies \( l(x) \leq l(x^*) + \epsilon \).

Therefore, if predetermined \( k \) and \( \epsilon \) violate the above condition, the \( \epsilon \)-error guarantee cannot be obtained. If we are to obtain guarantees that hold with any \( k \), one naive approach is the exhaustive search; i.e., we solve \( \min_{\text{supp}(x') \subseteq S} l(x) \) for all \( S \subseteq [d] \) of size \( k \), which incurs \( \Omega(d^k) \) computation cost. Bertsimas et al. [2] showed that problem (2) can be solved via mixed-integer programming (MIP) if \( l(\cdot) \) is quadratic, but the resulting MIP is generally as hard as the original problem. These results are not strong enough in terms of computational complexity, and so the following question naturally arises. Given any \( k \) and \( \epsilon \), can we compute an \( \epsilon \)-error solution, \( x \), that satisfies \( \|x\|_0 \leq k \) without requiring \( \Omega(d^k) \) computation cost?

To answer this question, we use the parametrized complexity framework [9]. We regard a part of the input as fixed parameter(s), which is denoted by \( p \) and does not include instance size \( d \). Our aim is to design an algorithm that runs in \( g(p) \cdot \text{poly}(d) \) time, where \( g(\cdot) \) is some computable function of \( p \). Such algorithms are said to be fixed-parameter tractable (FPT). Note that, if \( k \) is a fixed parameter, algorithms that require \( \Omega(d^k) \) time (e.g., exhaustive search) are not FPT. In this section, regarding \( k \) as a part of the fixed parameters, we obtain **Rand-FPT-Approx** for weakly modular maximization (1). Thanks to Proposition 1 this result gives a randomized FPT \( \epsilon \)-error algorithm for \( \ell_0 \)-constrained minimization (2).

**Theorem 2.** Assume that \( F \) is monotone and \( (\gamma_{k,k}, \gamma_{k,d}) \)-weakly modular. Let \( S^* \) be an optimal solution for problem (1). For any \( \epsilon > 0 \), if Algorithm 1 runs with

\[ T \geq \left\lceil \left( \frac{1}{\gamma_{k,k} \gamma_{k,d}} \cdot \frac{1 + \epsilon}{\epsilon} \right)^k \log \delta^{-1} \right\rceil, \]

then the obtained solution \( S \) satisfies \( F(S) \geq (1 + \epsilon)F(S^*) - \epsilon F([d]) \) with a probability of at least \( 1 - \delta \).
Algorithm 2 Multi-stage algorithm

1: $U \leftarrow [d]$, $S \leftarrow \emptyset$
2: for $i = 1, \ldots, m$ do
3: \quad $B_i \leftarrow \arg \max_{B \subseteq U : |B| \leq b_i} G_S(B)$
4: \quad $S \leftarrow S \cup B_i$
5: \quad $U \leftarrow U \setminus B_i$
6: return $S$

Therefore, if $F(\cdot)$ can be evaluated in poly($d$) time as assumed in Section 2.1 and $p := (k, \gamma, k, \gamma_{k,d}, \epsilon, \delta)$ are regarded as fixed parameters, then Algorithm 1 is FPT. We remark that this result does not contradict Theorem 1 for the following reason: Theorem 1 is obtained by using a $k$ value that increases with $d$ (see, the appendix), and such a $k$ cannot be regarded as a fixed parameter.

We turn to problem (2). Thanks to Theorem 2 and Proposition 1 we obtain the following guarantee.

**Corollary 2.1.** Suppose that $F(\cdot)$ is defined by (3), where $l(\cdot)$ is assumed to be $\mu_{2k}$-RSC, $\mu_{k+1}$-RSC, $\nu_{k+1,1}$-RSM, and $\nu_d$-RSM. Let $x^*$ be an optimal solution for problem (2) and define $l := l(x^*) - \min_{x \in \mathbb{R}^d} l(x)$. If Algorithm 2 runs with

$$T \geq \left[ \left( \frac{\nu_{k+1,1}}{\mu_{2k}}, \frac{\nu_d}{\mu_{k+1}}, \frac{l + \epsilon}{\epsilon} \right) \right]^{k} \log \delta^{-1}$$

and outputs $S$, then $x = \arg \min_{\supp(x') \subseteq S} l(x')$ satisfies $\|x\|_0 \leq k$ and achieves $l(x) \leq l(x^*) + \epsilon$ with a probability of at least $1 - \delta$.

Since $F(\cdot)$ is assumed to be evaluated in poly($d$) time, this result means that Algorithm 1 can compute $\epsilon$-error solutions with high probability in FPT time, where we regard $p := (k, \mu_{2k}, \mu_{k+1}, \nu_{k+1,1}, \nu_d, l, \epsilon, \delta)$ as fixed parameters. Note that Corollary 2.1 holds for any $k$ unlike Proposition 4.

5 Multi-stage Algorithms

When applying greedy-style algorithms to large-scale instances, the growth of computation cost causes a bottleneck. For example, *Greedy* requires us to evaluate $F(\cdot)$ up to $d$ times in each iteration; if $F(\cdot)$ is defined as in (2), we need to repeatedly solve the minimization problems. To alleviate such increases in computation cost, we can use the multi-stage approach. With this approach, we add multiple elements in each iteration, thus making the algorithm terminate quickly. In this section, we first prove a guarantee of *Multi-Greedy* for weakly modular maximization; as a corollary, we obtain its guarantee for $\ell_0$-constrained minimization. We then prove a guarantee of *Multi-OMP* for $\ell_0$-constrained minimization. We finally confirm their practical advantages via experiments. In this section, we take $S^*$ and $x^*$ to be target solutions for problems (1) and (2), respectively, and define $k^* := |S^*| = \|x^*\|_0$. This enables us to obtain guarantees even if $k \neq k^*$.

Algorithm 2 is the framework for multi-stage algorithms. The algorithm continues $m$ iterations ($m \leq k$) to obtain a solution. In each $i$-th iteration ($i \in [m]$), we choose a subset $B_i \subseteq [d]$ of size at most $b_i \geq 1$. The subset, $B_i$, is chosen so that it maximizes a surrogate function, $G_S(\cdot)$, where $S$ is the current solution. Here, we suppose $G_S$ to be monotone, and so we have $|B_i| = b_i$ for each $i \in [m]$. To obtain efficient multi-stage algorithms, $G_S$ should be evaluated and maximized efficiently. The design of $G_S$ determines whether Algorithm 2 becomes *Multi-Greedy* or *Multi-OMP*, which we detail below.

5.1 Multi-Greedy

*Multi-Greedy* uses the following surrogate function:

$$G_S(B) = \sum_{j \in B} F(j \mid S).$$

A similar surrogate function was considered by Wei et al. [38], and they proved an approximation guarantee for the case where $F(\cdot)$ is monotone and submodular; roughly speaking, their approximation factor is $2/(1 - e^{-\alpha(1 - \alpha)})$, which is equal to 0 if $\alpha = 1$. Taking Proposition 3 into account, if we consider applying *Multi-Greedy* to $\ell_0$-constrained minimization, we need to prove its approximation guarantee for weakly modular $F(\cdot)$ without using its curvature. Fortunately, it can be proved as shown below. Let $S_i$ be the solution obtained after the $i$-th iteration; $S_m$ is the output. Then the following theorem holds:
Theorem 3. Let \( b_{\min}, b_{\max} \) be integers such that \( 0 < b_{\min} \leq b_{\max} \leq k^* \). Set \( b_1, \ldots, b_m \) so as to satisfy \( b_i \in [b_{\min}, b_{\max}] \) for \( i \in [m] \) and \( \sum_{i=1}^{m} b_i = k \). If \( F \) is \( (\gamma_{s_m, k^*}, \gamma_{s_m, b_{\max}}) \)-weakly modular, solution \( S_m \) obtained with Multi-Greedy satisfies

\[
F(S_m) \geq \left( 1 - \exp \left( -\gamma_{s_m, k^*} \frac{k}{\lambda_{k^*}} \right) \right) F(S^*).
\]

If we set \( b_{\min} = b_{\max} = 1 \), the above result recovers the \((1 - e^{-\gamma_{s_m, 1}})\)-approximation guarantee of Greedy for weakly submodular maximization [10] since \( \gamma_{s_m, 1} = 1 \). By defining \( F \) as in (3) and using Theorem 3 and Proposition 1, we obtain the following guarantee of Multi-Greedy for \( \ell_0 \)-constrained minimization (2):

Corollary 3.1. Let \( x = \arg \min_{\supp(x') \subseteq S_m} l(x') \), where \( S_m \) is the output of Multi-Greedy. If \( l(\cdot) \) has restricted condition numbers \( \kappa_{k+1} \) and \( \kappa_{k+k^*} \), we have

\[
l(x) \leq l(x^*) + \exp \left( -\frac{1}{\kappa_{k+1} \kappa_{k+k^*}} \frac{k}{\lambda_{k^*}} \right) (l(0) - l(x^*)�).
\]

5.2 Multi-OMP

We then consider Multi-OMP for \( \ell_0 \)-constrained minimization [2], which uses the following surrogate function:

\[
G_S(B) = \| \nabla l(b(\cdot)) \|_2 = \sum_{j \in B} |\nabla l(b(\cdot))_j|^2,
\]

where \( b(\cdot) = \arg \min_{\supp(x') \subseteq S} l(x') \). As in [12], if we choose \( \arg \max_{j \in B} |\nabla l(b(\cdot))_j|^2 \) in each iteration, the algorithm coincides with OMP. A similar multi-stage algorithm was proposed by Marsousi et al. [25] for the case where \( l(\cdot) \) is quadratic, but its theoretical guarantee has not been proved. By using Lemma 1, we can obtain the following guarantee of Multi-OMP, which is better than that of Multi-Greedy (Corollary 3.1):

Theorem 4. Set \( b_1, \ldots, b_m \) as in Theorem 3 and assume that \( l(\cdot) \) is \( \mu_{k+k^*} \)-RSC and \( \nu_{k,b_{\max}} \)-RSM. If \( S_m \) is a solution of Multi-OMP, \( x = \arg \min_{\supp(x') \subseteq S_m} l(x') \) satisfies

\[
l(x) \leq l(x^*) + \exp \left( -\frac{\mu_{k+k^*}}{\nu_{k,b_{\max}}} \frac{k}{\lambda_{k^*}} \right) (l(0) - l(x^*)) ≤ l(x^*) + \exp \left( -\frac{1}{\kappa_{k+k^*}} \frac{k}{\lambda_{k^*}} \right) (l(0) - l(x^*)�).
\]

We can readily check that this result matches those obtained for OMP and Greedy shown in [12] (see also Proposition 4). Namely, the use of the multi-stage approach does not degrade the theoretical guarantee.

In practice, the surrogate function of Multi-OMP is often easier to compute than that of Multi-Greedy, and so Multi-OMP is typically faster than Multi-Greedy. On the other hand, as we will see in the experiments, Multi-Greedy empirically outperforms Multi-OMP as regards solution quality, which is contrary to the above theoretical results. It will be interesting future work to study this gap between theory and practice.

5.3 Experiments

We evaluate Multi-Greedy and Multi-OMP via experiments with \( \ell_0 \)-constrained minimization instances. As baseline methods, we used IHT and HTP, where we continued their iterations until the objective-value improvement, \( l(x_i) - l(x_{i+1}) \), became smaller than \( 10^{-5} \). We also applied standard Greedy and OMP to the instances. All the algorithms were implemented in Python 3.6.6 and all the experiments were conducted on a 64-bit macOS (High Sierra) machine with 3.3GHz Intel Core i7 CPUs and 16 GB RAM.
Figure 3: Semi-log plots of running times, training errors, and test errors for real-world instances with various $k$.

5.3.1 Synthetic Instances

Settings. We consider well- and ill-conditioned synthetic instances of estimating $x \in \mathbb{R}^d$ such that $\|x\|_0 = k$ from a sample of size $n$. Given design matrix $A \in \mathbb{R}^{n \times d}$ and observation vector $y \in \mathbb{R}^n$, we use a quadratic loss function: $l(x) := \frac{1}{2\gamma}\|y - Ax\|_2^2$. We randomly generated well- and ill-conditioned instances as follows: We set $k$ entries of the true sparse solution, $x_{\text{true}}$, at 1 and the others at 0, where the $k$ entries were chosen uniformly at random. In the well-conditioned case, we drew each entry of $A$ from the standard normal distribution, denoted by $\mathcal{N}$. In the ill-conditioned case, we drew each row of $A$ from a heavily correlated $d$-dimensional normal distribution, whose correlation coefficient was set at 0.8. We then set $y = Ax_{\text{true}} + 0.1u$, where each entry of $u \in \mathbb{R}^n$ was drawn from $\mathcal{N}$. We consider various dimensionalities: $d = 200, 400, \ldots, 1000$. We let $k = 0.1d$ and $n = \lfloor 5k \log d \rfloor$. We randomly generated 100 instances for each $d$.

Results. The running times and objective values achieved with each method are shown in Figure 2, where each value is calculated by taking an average over 100 instances. Multi-Greedy-$b$ and Multi-OMP-$b$ represent the multi-stage algorithms that choose $B_i$ of size $b$ in each iteration. For example, if $b = 0.1k$, the algorithms terminate after 10 iterations; Greedy and OMP correspond to Multi-Greedy-$1$ and Multi-OMP-$1$, respectively. In all cases, the multi-stage algorithms speed up as $b$ increases. In the well-conditioned case, Multi-OMP-$0.5k$ is the fastest, and all methods achieve the same objective values, implying that the instances are easy enough. In the ill-conditioned case, we see that the parameter, $b$, of multi-stage algorithms controls the trade-off between the running times and objective values. Multi-Greedy-$0.5k$ (Multi-OMP-$0.5k$) is faster than IHT (HTP), and the objective values of Multi-Greedy and Multi-OMP are better than those of IHT and HTP. To conclude, by setting the size of $B_i$ appropriately, multi-stage algorithms can outperform projected-gradient-based methods (IHT and HTP) both in running time and solution quality. All of the algorithms can be accelerated via randomization [24, 22], but, to simplify the comparisons, we did not consider such techniques.

5.3.2 Real-world Instances

Settings. We again consider sparse regression instances. To obtain $A$ and $y$, we used the “satellite_image” dataset, which is available at PMLB. We used the 1st and 2nd order polynomial features; as a result, the dataset has $d = 666$ features and a sample of size $n = 6435$. We split the sample into training data ($n = 3435$) and test data ($n = 3000$). We considered various values of sparsity: $k = 20, 40, \ldots, 100$. With each $k$ value, we evaluated the algorithms based on running times, training errors, and test errors.

Results. The results are summarized in Figure 3 Here, Multi-Greedy-$b$ and Multi-OMP-$b$ represent the multi-stage algorithms that choose $B_i$ of size at least $b$ in each iteration. As with the results obtained with synthetic data, the multi-stage algorithms speed up as $b$ increases. In particular, Multi-OMP-$0.1k$ is faster and achieves smaller training and test errors than IHT/HTP. Multi-Greedy-$0.1k$ is faster than IHT except when $k = 40$, and its errors are particularly small (almost the same as those of Greedy). These results demonstrate the practical advantages of the multi-stage algorithms.

6 Conclusion

We made theoretical and practical contributions to weakly modular maximization. We proved the hardness of improving the $(1 - e^{-\gamma k})$-approximation guarantee for a certain class of problems. We presented Rand-FPT-Approx for weakly modular maximization. As a corollary, we obtained a randomized FPT $\epsilon$-error algorithm for $\ell_0$-constrained
minimization. We proved guarantees of Multi-Greedy and Multi-OMP. We experimentally confirmed that these methods can run faster and find better solutions than IHT/HTP, particularly when instances are ill-conditioned.

Recent studies [22, 31] have provided various techniques for accelerating greedy algorithms, and greedy-style methods for many different settings have also been studied [35, 5, 16]. It will be interesting future work to study how to incorporate the multi-stage approach into those methods for further acceleration.

References

[1] Bai, W. and Bilmes, J. Greed is still good: Maximizing monotone Submodular+Supermodular (BP) functions. In *Proceedings of the 35th International Conference on Machine Learning*, volume 80, pp. 304–313. PMLR, 2018.

[2] Bertsimas, D., King, A., and Mazumder, R. Best subset selection via a modern optimization lens. *Ann. Statist.*, 44(2): 813–852, 2016.

[3] Bian, A. A., Buhmann, J. M., Krause, A., and Tschatschek, S. Guarantees for greedy maximization of non-submodular functions with applications. In *Proceedings of the 34th International Conference on Machine Learning*, volume 70, pp. 498–507. PMLR, 2017.

[4] Blumensath, T. and Davies, M. E. Iterative hard thresholding for compressed sensing. *Appl. Comput. Harmon. Anal.*, 27(3):265–274, 2009.

[5] Bogunovic, I., Zhao, J., and Cevher, V. Robust maximization of non-submodular objectives. In *Proceedings of the 21st International Conference on Artificial Intelligence and Statistics*, volume 84 of *Proceedings of Machine Learning Research*, pp. 890–899. PMLR, 2018.

[6] Candès, E. J., Romberg, J. K., and Tao, T. Stable signal recovery from incomplete and inaccurate measurements. *Comm. Pure Appl. Math.*, 59(8):1207–1223, 2006.

[7] Chen, L., Feldman, M., and Karbasi, A. Weakly submodular maximization beyond cardinality constraints: Does randomization help greedy? In *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pp. 804–813. PMLR, 2018.

[8] Conforti, M. and Cornuéjols, G. Submodular set functions, matroids and the greedy algorithm: Tight worst-case bounds and some generalizations of the Rado-Edmonds theorem. *Discrete Appl. Math.*, 7(3):251–274, 1984.

[9] Cygan, M., Fomin, F. V., Kowalik, L., Lokshtanov, D., Marx, D., Pilipczuk, M., Pilipczuk, M., and Saurabh, S. *Parameterized Algorithms*. Springer Publishing Company, Incorporated, 1st edition, 2015.

[10] Das, A. and Kempe, D. Submodular meets spectral: Greedy algorithms for subset selection, sparse approximation and dictionary selection. In *Proceedings of the 28th International Conference on Machine Learning*, pp. 1057–1064. ACM, 2011.

[11] Elenberg, E. R., Dimakis, A. G., Feldman, M., and Karbasi, A. Streaming weak submodularity: Interpreting neural networks on the fly. In *Advances in Neural Information Processing Systems 30*, pp. 4044–4054. Curran Associates, Inc., 2017.

[12] Elenberg, E. R., Khanna, R., Dimakis, A. G., and Negahban, S. Restricted strong convexity implies weak submodularity. *Ann. Statist.*, 46(6B):3539–3568, 2018.

[13] Feige, U. A threshold of ln n for approximating set cover. *J. ACM*, 45(4):634–652, 1998.

[14] Feige, U. and Izsak, R. Welfare maximization and the supermodular degree. In *Proceedings of the 4th Conference on Innovations in Theoretical Computer Science*, pp. 247–256. ACM, 2013.

[15] Foucart, S. Hard thresholding pursuit: An algorithm for compressive sensing. *SIAM J. Optim.*, 49(6):2543–2563, 2011.

[16] Fujii, K. and Soma, T. Fast greedy algorithms for dictionary selection with generalized sparsity constraints. In *Advances in Neural Information Processing Systems 31*, pp. 4749–4758. Curran Associates, Inc., 2018.

[17] Horel, T. and Singer, Y. Maximization of approximately submodular functions. In *Advances in Neural Information Processing Systems 29*, pp. 3045–3053. Curran Associates, Inc., 2016.

[18] Iyer, R. K., Jegelka, S., and Bilmes, J. A. Curvature and optimal algorithms for learning and minimizing submodular functions. In *Advances in Neural Information Processing Systems 26*, pp. 2742–2750. Curran Associates, Inc., 2013.

[19] Jain, P. and Kar, P. Non-convex optimization for machine learning. *Foundations and Trends® in Machine Learning*, 10(3-4):142–336, 2017.
[20] Jain, P., Tewari, A., and Kar, P. On iterative hard thresholding methods for high-dimensional M-estimation. In *Advances in Neural Information Processing Systems 27*, pp. 685–693. Curran Associates, Inc., 2014.

[21] Khanna, R., Elenberg, E. R., Dimakis, A. G., Ghosh, J., and Negahban, S. On approximation guarantees for greedy low rank optimization. In *Proceedings of the 34th International Conference on Machine Learning*, volume 70, pp. 1837–1846. PMLR, 2017.

[22] Khanna, R., Elenberg, E. R., Dimakis, A. G., Negahban, S., and Ghosh, J. Scalable greedy feature selection via weak submodularity. In *Proceedings of the 20th International Conference on Artificial Intelligence and Statistics*, volume 54, pp. 1560–1568. PMLR, 2017.

[23] Krause, A. and Cevher, V. Submodular dictionary selection for sparse representation. In *Proceedings of the 27th International Conference on International Conference on Machine Learning*, pp. 567–574. Omnipress, 2010.

[24] Li, X., Zhao, T., Arora, R., Liu, H., and Haupt, J. Stochastic variance reduced optimization for nonconvex sparse learning. In *Proceedings of the 33rd International Conference on Machine Learning*, volume 48, pp. 917–925. PMLR, 2016.

[25] Liberty, E. and Sviridenko, M. Greedy minimization of weakly supermodular set functions. In *Proceedings of Approximation, Randomization, and Combinatorial Optimization. Algorithms and Techniques*, volume 81, pp. 19:1–19:11. Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, 2017.

[26] Marsousi, M., Abhari, K., Babyn, P., and Alirezaie, J. MULTI-STAGE OMP sparse coding using local matching pursuit atoms selection. In *2013 IEEE International Conference on Acoustics, Speech and Signal Processing*, pp. 1783–1787, 2013.

[27] Natarajan, B. K. Sparse approximate solutions to linear systems. *SIAM J. Optim.*, 24(2):227–234, 1995.

[28] Nemhauser, G. L. and Wolsey, L. A. Best algorithms for approximating the maximum of a submodular set function. *Math. Oper. Res.*, 3(3):177–188, 1978.

[29] Nemhauser, G. L., Wolsey, L. A., and Fisher, M. L. An analysis of approximations for maximizing submodular set functions-I. *Math. Program.*, 14(1):265–294, 1978.

[30] Pati, Y. C., Rezaifar, R., and Krishnaprasad, P. S. Orthogonal matching pursuit: recursive function approximation with applications to wavelet decomposition. In *Proceedings of the 27th Asilomar Conference on Signals, Systems and Computers*, pp. 40–44 vol.1, 1993.

[31] Qian, C., Yu, Y., and Tang, K. Approximation guarantees of stochastic greedy algorithms for subset selection. In *Proceedings of the 27th International Joint Conference on Artificial Intelligence*, pp. 1478–1484. International Joint Conferences on Artificial Intelligence Organization, 7 2018.

[32] Shalev-Shwartz, S. and Zhang, T. Accelerated proximal stochastic dual coordinate ascent for regularized loss minimization. *Math. Program.*, 155(1):105–145, 2016.

[33] Shalev-Shwartz, S., Srebro, N., and Zhang, T. Trading accuracy for sparsity in optimization problems with sparsity constraints. *SIAM J. Optim.*, 20(6):2807–2832, 2010.

[34] Skowron, P. FPT approximation schemes for maximizing submodular functions. *Inform. Comput.*, 257:65 – 78, 2017.

[35] Stan, S., Zadimoghaddam, M., Krause, A., and Karbasi, A. Probabilistic submodular maximization in sub-linear time. In *Proceedings of the 34th International Conference on Machine Learning*, volume 70, pp. 3241–3250. PMLR, 2017.

[36] Sviridenko, M., Vondrák, J., and Ward, J. Optimal approximation for submodular and supermodular optimization with bounded curvature. In *Proceedings of the 26th Annual ACM-SIAM Symposium on Discrete Algorithms*, pp. 1134–1148. SIAM, 2015.

[37] Vondrak, J. Optimal approximation for the submodular welfare problem in the value oracle model. In *Proceedings of the Fortieth Annual ACM Symposium on Theory of Computing*, pp. 67–74. ACM, 2008.

[38] Wei, K., Iyer, R., and Bilmes, J. Fast multi-stage submodular maximization. In *Proceedings of the 31st International Conference on Machine Learning*, volume 32, pp. 1494–1502. PMLR, 22–24 Jun 2014.

[39] Yuan, X., Li, P., and Zhang, T. Exact recovery of hard thresholding pursuit. In *Advances in Neural Information Processing Systems 29*, pp. 3558–3566. Curran Associates, Inc., 2016.
Appendix

In Section A, we show that RSC and RSM imply weak modularity. In Section B, we present an \( l_q \)-constrained minimization instance such that the curvature and inverse curvature of \( F(\cdot) \) are 1 while \( l(\cdot) \) has a bounded condition number, which means that the submodularity and supermodularity ratios of \( F(\cdot) \) are bounded. In Section C, we present the proof of the hardness result. In Section D, we prove the guarantee of the FPT algorithm. In Section E, we prove the guarantees of the multi-stage algorithms.

A RSC and RSM Imply Weak Modularity

For convenience, we define \( f(x) := l(0) - l(x) \) in what follows. Note that we have \( F(S) = l(0) - \min_{\text{supp}(x) \subseteq S} l(x) = \max_{\text{supp}(x) \subseteq S} f(x) \) for any \( S \subseteq \mathbb{R}^d \). If \( l(\cdot) \) is \( \mu_\Omega \)-RSC and \( \nu_\Omega \)-RSM, then \( f(\cdot) \) has \( \mu_\Omega \)-restricted strong concavity (\( \mu_\Omega \)-RSC) and \( \nu_\Omega \)-restricted smoothness (\( \nu_\Omega \)-RSM) as follows:

\[
-\frac{\mu_\Omega}{2} \|y - x\|^2 \geq f(y) - f(x) - \langle \nabla f(x), y - x \rangle \geq -\frac{\nu_\Omega}{2} \|y - x\|^2
\]

for any \( (x, y) \in \Omega \). We introduce the following definitions:

- If \([A1]\) holds with \( \Omega = \Omega_{k_1, k_2} := \{ (x, y) \mid \|x\| \leq k_1, \|y\| \leq k_1, \|x - y\| \leq k_2 \} \), we say \( f(\cdot) \) is \( \mu_{k_1, k_2} \)-RSC and \( \nu_{k_1, k_2} \)-RSM. For simplicity, we define \( \mu_k := \mu_{k,k} \) and \( \nu_k := \nu_{k,k} \).

- Given \( A, B \subseteq \mathbb{R}^d \), if \([A1]\) holds with \( \Omega = \Omega_{A,B} := \{ (x, y) \mid \text{supp}(x) \subseteq A, \text{supp}(y) \subseteq B \} \), we say \( f(\cdot) \) is \( \mu_{A,B} \)-RSC and \( \nu_{A,B} \)-RSM.

- Given \( A \subseteq B \subseteq \mathbb{R}^d \), if \([A1]\) holds with \( \Omega = \Omega_{A,B} := \{ (x, y) \mid \text{supp}(x) \subseteq A, \text{supp}(y) \subseteq B, \text{supp}(y - x) \subseteq B \setminus A \} \), we say \( f(\cdot) \) is \( \tilde{\mu}_{A,B} \)-RSC and \( \tilde{\nu}_{A,B} \)-RSM.

For \( \Omega' \subseteq \Omega \), we can set \( \mu_{\Omega'} \) and \( \nu_{\Omega'} \) so that we have \( \mu_{\Omega'} \geq \mu_\Omega \) and \( \nu_{\Omega'} \leq \nu_\Omega \), respectively. In particular, we often use the following inequalities:

- For any \( 0 \leq k'_1 \leq k_1 \) and \( 0 \leq k'_2 \leq k_2 \) we have \( \mu_{k_1, k_2} \leq \mu_{k'_1, k'_2} \) and \( \nu_{k_1, k_2} \geq \nu_{k'_1, k'_2} \).

- For any \( A, B \subseteq \mathbb{R}^d \), we have \( \mu_{|A,B|} \leq \mu_{A,B} \) and \( \nu_{|A,B|} \geq \nu_{A,B} \).

- For any \( A \subseteq B \subseteq \mathbb{R}^d \), we have \( \mu_{|B| \setminus A} \leq \tilde{\mu}_{A,B} \) and \( \nu_{|B| \setminus A} \geq \tilde{\nu}_{A,B} \).

The following lemma, whose weaker version is presented in the main paper, is the key to proving Proposition 1.

**Lemma 1** (implied in [12]). For any \( A \subseteq \mathbb{R}^d \), let \( b^{(A)} := \arg\max_{\text{supp}(x) \subseteq A} f(x) \). Then, for any disjoint \( A, B \subseteq \mathbb{R}^d \), if \( f(\cdot) \) is \( \mu_{A,A,B} \)-RSC and \( \nu_{A,A,B} \)-RSM, we have

\[
\frac{1}{2\mu_{A,A,B}} \|\nabla f(b^{(A)})\|_{B}^2 \leq F(B \mid A) \leq \frac{1}{2\nu_{A,A,B}} \|\nabla f(b^{(A)})\|_{B}^2.
\]

**Proof.** We show the first inequality. Since \( b^{(A \cup B)} \) is the maximizer of \( f(\cdot) \) over \( \{ x \in \mathbb{R}^d \mid \text{supp}(x) \subseteq A \cup B \} \), we have \( f(b^{(A \cup B)}) \geq f(w + b^{(A)}) \) for any \( \text{supp}(w) \subseteq B \). Therefore, from the inequality of RSM, we obtain

\[
F(B \mid A) = f(b^{(A \cup B)}) - f(b^{(A)}) \geq f(w + b^{(A)}) - f(b^{(A)})
\]

\[
\geq \langle \nabla f(b^{(A)}), w \rangle - \frac{\nu_{A,A,B}}{2} \|w\|_{B}^2.
\]

Setting \( w_B = \frac{1}{\nu_{A,A,B}} \nabla f(b^{(A)})_B \) and \( w_{\mathbb{R}^d \setminus B} = 0 \), we obtain the first inequality:

\[
F(B \mid A) \geq \frac{1}{2\nu_{A,A,B}} \|\nabla f(b^{(A)})\|_{B}^2.
\]

We then prove the second inequality. Thanks to the inequality of RSC, we have

\[
F(B \mid A) = f(b^{(A \cup B)}) - f(b^{(A)})
\]

\[
\leq \langle \nabla f(b^{(A)}), b^{(A \cup B)} - b^{(A)} \rangle - \frac{\mu_{A,A,B}}{2} \|b^{(A \cup B)} - b^{(A)}\|_{2}^2.
\]
Let \( \mathbf{w} \in \mathbb{R}^{|d|} \) be a vector such that \( \text{supp}(\mathbf{w}) \subseteq \mathbf{A} \cup \mathbf{B} \). We consider replacing \( \mathbf{b}^{(A:B)} \) in RHS with \( \mathbf{w} + \mathbf{b}^{(A)} \) and maximizing RHS w.r.t. \( \mathbf{w} \); we thus obtain an upper bound of \( F(\mathbf{B} | A) \) as follows:

\[
F(\mathbf{B} | A) \leq \max_{\text{supp}(\mathbf{w}) \subseteq \mathbf{A} \cup \mathbf{B}} \langle \nabla f(\mathbf{b}^{(A)}), \mathbf{w} \rangle - \frac{\mu_{A,A:B}}{2} \|\mathbf{w}\|_2^2.
\]

The maximum is attained with \( \mathbf{w}_{A:B} = \frac{1}{\mu_{A,A:B}} \nabla f(\mathbf{b}^{(A)})_{A:B} \), and so we obtain

\[
F(\mathbf{B} | A) \leq \frac{1}{2\mu_{A,A:B}} \|\nabla f(\mathbf{b}^{(A)})_{A:B}\|_2^2 = \frac{1}{2\mu_{A,A:B}} \|\nabla f(\mathbf{b}^{(A)})_{B}\|_2^2,
\]

where the last equality comes from the first-order optimality condition (or the KKT condition with the linear independence constraint qualification) at \( \mathbf{b}^{(A)} \): \( \nabla f(\mathbf{b}^{(A)})_{A} = 0 \). \( \square \)

Below we prove Proposition 1 using the above lemma.

**Proposition 1** (partially adopted from [12, 5]). For any \( \mathbf{U} \subseteq [d] \) and \( k \in \mathbb{Z}_{>0} \), submodularity ratio \( \gamma_{U,k} \) and supermodularity ratio \( \bar{\gamma}_{U,k} \) of \( F(\cdot) \) are bounded with RSC and RSM constants of \( l(\cdot) \) as follows:

\[
\begin{align*}
\gamma_{U,k} & \geq \frac{\mu_{|U|+k}}{\nu_{|U|+1}} \geq \frac{\mu_{|U|+k}}{\nu_{|U|+k}} = \frac{1}{\kappa_{|U|+k}}, \\
\bar{\gamma}_{U,k} & \geq \frac{\mu_{|U|+1}}{\nu_{|U|+k,k}} \geq \frac{\mu_{|U|+1}}{\nu_{|U|+k}} = \frac{1}{\kappa_{|U|+k}}.
\end{align*}
\]

**Proof.** We refer the readers to [12] for the proof of the lower bound of \( \gamma_{U,k} \). Here, we show how to obtain the lower bound of \( \bar{\gamma}_{U,k} \). From the definition of the supermodularity ratio, we have

\[
\bar{\gamma}_{U,k} := \min_{L, S : L \cap S = \emptyset, L \subseteq \mathbf{U}, |S| \leq k} \frac{F(S | L)}{\sum_{j \in S} F(j | L)}.
\]

where we regard \( 0/0 = 1 \). Therefore, we obtain

\[
\bar{\gamma}_{U,k} \geq \min_{L, S : L \cap S = \emptyset, L \subseteq \mathbf{U}, |S| \leq k} \left\| \nabla f(\mathbf{b}^{(L)})_{S}\right\|_2^2 \left( \sum_{j \in S} \left\| \nabla f(\mathbf{b}^{(L)})_{j}\right\|_2^2 \right)^{-1} \quad \therefore \text{Lemma 1}
\]

\[
\geq \min_{L, S : L \cap S = \emptyset, L \subseteq \mathbf{U}, |S| \leq k} \frac{\mu_{|U|+1}}{\nu_{L,U:S}} \left( \sum_{j \in S} \left\| \nabla f(\mathbf{b}^{(L)})_{j}\right\|_2^2 \right) \quad \therefore \mu_{L,U:S(j)} \geq \mu_{|U|+1}
\]

\[
\geq \min_{L, S : L \cap S = \emptyset, L \subseteq \mathbf{U}, |S| \leq k} \frac{\mu_{|U|+1}}{\nu_{L,U:S}} \quad \therefore \|
abla f(\mathbf{b}^{(L)})_{S}\|_2^2 = \sum_{j \in S} |\nabla f(\mathbf{b}^{(L)})_{j}|^2
\]

The proof is completed with \( \nu_{|U|+k,k} \leq \nu_{|U|+k} \) and \( \mu_{|U|+1} \geq \mu_{|U|+k} \). \( \square \)

**B \quad \ell_0\text{-constrained Minimization Instance with a Bounded Condition Number and Unbounded Curvatures}**

We show that there is an instance of form \( \min_{\mathbf{x} \in \mathbb{R}^{[d]} : \|\mathbf{x}\|_0 \leq k} l(\mathbf{x}) \) that satisfies following conditions: Condition number \( \kappa \) of \( l(\cdot) \) is bounded by a constant, while curvature \( \alpha \) and inverse curvature \( \alpha \) of \( F(S) = l(0) - \min_{\supp(\mathbf{x}) \subseteq S} l(\mathbf{x}) \) are equal to 1.

We define

\[
\mathbf{B} := \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{a}_1 := \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \text{and} \quad \mathbf{a}_2 := \begin{bmatrix} 1 \\ 1 \end{bmatrix}.
\]
Note that we have
\[
\begin{align*}
\min_{x_1, x_2 \in \mathbb{R}} \left\| B \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - a_1 \right\|_2^2 &= 0, \\
\min_{x_1 \in \mathbb{R}} \left\| B \begin{bmatrix} x_1 \\ 0 \end{bmatrix} - a_1 \right\|_2^2 &= 1, \\
\min_{x_3, x_4 \in \mathbb{R}} \left\| B \begin{bmatrix} x_3 \\ x_4 \end{bmatrix} - a_2 \right\|_2^2 &= 0, \\
\min_{x_3 \in \mathbb{R}} \left\| B \begin{bmatrix} x_3 \\ 0 \end{bmatrix} - a_2 \right\|_2^2 &= 1/2, \\
\min_{x_1, x_2 \in \mathbb{R}} \left\| B \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - a_1 \right\|_2^2 &= 1/2, \\
\min_{x_3, x_4 \in \mathbb{R}} \left\| B \begin{bmatrix} x_3 \\ x_4 \end{bmatrix} - a_2 \right\|_2^2 &= 0.
\end{align*}
\]

We define the objective function as \( l(x) := \| Ax - y \|_2^2 \), where \( A \in \mathbb{R}^{[d] \times [d]} \) is a block-diagonal matrix and \( y \in \mathbb{R}^{[d]} \) is a vector defined as
\[
A := \begin{bmatrix} B & B & \cdots & B \\ & 1 \\ & & \ddots \\ & & & 1 \end{bmatrix}
\quad \text{and} \quad y := \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ 0 \end{bmatrix},
\]
respectively. We let \( F(S) = l(0) - \min_{\text{supp}(x) \subseteq S} l(x) \) for any \( S \subseteq [d] \). Then we have
\[
F(\{1\} \mid \{2\}) = 1/2, \quad F(\{1\}) = 0, \quad F(\{3\} \mid \{4\}) = 0, \quad \text{and} \quad F(\{3\}) = 1.
\]
Since \( \alpha, \alpha \in [0, 1] \) must satisfy
\[
F(\{1\}) \geq (1 - \alpha) F(\{1\} \mid \{2\}) \quad \text{and} \quad F(\{3\} \mid \{4\}) \geq (1 - \alpha) F(\{3\}),
\]
we have \( \alpha = \alpha = 1 \). On the other hand, the condition number, \( \kappa \), of \( l(\cdot) \) is bounded from above by the ratio of the largest and smallest eigenvalues of \( A^T A \), which are equal to \( \frac{3 + \sqrt{5}}{2} \) and \( \frac{3 - \sqrt{5}}{2} \), respectively; hence \( \kappa \leq \frac{3 + \sqrt{5}}{3 - \sqrt{5}} \).

C Hardness Result

We prove the hardness result based on the idea presented in [28]. By designing objective function \( F \) appropriately, we reduce the problem of achieving an approximation guarantee that exceeds \( 1 - e^{-\gamma_{k,k}} \) to a problem of finding \( S \subseteq [d] \) such that \( |S \cap M| \geq r + 1 \) and \( |S| \leq p_k^k := 2k - r + 1 \), where \( M \) is an unknown subset of size \( k \) and \( r \leq k \) is any positive integer.

We explain how to design \( F(\cdot) \). Fix the unknown subset \( M \subseteq [d] \) of size \( k \). For any \( S \subseteq [d] \), we define the function value, \( F(S) \), so that it depends only on \( n_S := |S|, m_S := |S \cap M| \), \( r \) and \( k \). We denote such a function by \( G_k^k(m_S, n_S) \), and we let \( F(S) := G_k^k(|S \cap M|, |S|) = G_k^k(m_S, n_S) \). For any \( m \in [0, k] \) and \( n \in [0, d] \) such that \( m \leq n \), we define the value of \( G_k^k(m, n) \) so as to satisfy the following properties:

**Property 1:** \( F(\cdot) = G_k^k(\cdot, \cdot) \) is monotone, and its submodularity ratio \( \gamma_{k,k} \) and supermodularity ratio \( \hat{\gamma}_{k,k} \) satisfy
\[
\gamma_{k,k} = 1 \quad \text{and} \quad \hat{\gamma}_{k,k} = \left( 2 + \frac{r-1}{k-r+1} \right)^{-1},
\]
respectively.

**Property 2:** For any \( m \in [0, r] \) and \( n \in [0, d] \), the value of \( G_k^k(m, n) \) is independent of \( m \); i.e., \( G_k^k(0, n) = G_k^k(1, n) = \cdots = G_k^k(r, n) \).

**Property 3:** \( \max_{m, n, 0 \leq m \leq n \leq k} G_k^k(m, n) = G_k^k(k, k) = k(k - r + 1)^{k-r} \).

**Property 4:** For any \( n > p_k^k = 2k - r + 1 \) and \( m \in [0, k] \), we have \( G_k^k(m, n) = k(k - r + 1)^{k-r} \).

**Property 5:** \( G_k^k(0, k)/G_k^k(k, k) = 1 - \left( \frac{k-r+1}{k} \right) \left( \frac{k-r+1}{k} \right)^{k-r+1} = \alpha_k^{-1} \).

As in [28] Lemma 4.1, given monotone set function \( F(S) = G_k^k(m_S, n_S) \) that satisfies Properties 2–5, to achieve an approximation guarantee that exceeds \( \alpha_k^{-1} \) is at least as hard as the following problem:

For unknown \( M \subseteq [d] \) of size \( k \), find \( S \subseteq [d] \) that satisfies \( |S \cap M| \geq r + 1 \) and \( |S| \leq p_k^k \) by using the following feedback: Once \( S \) is proposed, we are informed whether or not \( S \) satisfies \( |S \cap M| \geq r + 1 \) and \( |S| \leq p_k^k \).

Intuitively, Properties 2 and 5 play crucial roles. If we are to achieve an approximation guarantee that exceeds \( \alpha_k^{-1} \), we need to find \( S \) such that \( n_S \geq r + 1 \), where the information of \( G_k^k \) values is worthless as long as \( n_S \leq r \). This fact gives a connection between the original problem and the above problem. Since \( M \) is unknown and no clue can be obtained by examining \( S \) that violates \( |S \cap M| \geq r + 1 \) or/and \( |S| \leq p_k^k \), the above problem cannot be solved via polynomially many queries. More precisely, the following proposition holds:
Proposition A1 (implied in the proof of [23, Theorem 4.2]). Consider the maximization problem of form \( \max_{S: |S| \leq k} F(S) \), where \( F(S) = G_r^k(m_S, n_S) \) has monotonicity and Properties 2–5. For this problem, to achieve an approximation guarantee that exceeds \( \alpha_k^{-1} \) requires us to evaluate \( F(\cdot) \) at least \( \Omega(d^{r+1}/k^{2r+2}) \) times.

By using the above properties and proposition, we obtain the main theorem.

Theorem 1. Consider a class of problems of form \( \max_{S: |S| \leq k} F(S) \) that satisfies the following conditions: \( F \) is monotone and has a submodularity ratio \( \gamma_{k,k} = 1 \) and a supermodularity ratio \( \gamma_{k,k} \geq 1/2 - \Theta(1/k) \) for \( k \geq 1/2 \). For this class, no algorithms that evaluate \( F(\cdot) \) only on polynomially many subsets can achieve an approximation guarantee that exceeds \( 1 - e^{-1} = 1 - e^{-\gamma_{k,k}} \).

Proof. The proof comprises two parts: (I) we prove the statement by assuming that there exists a function \( F(S) = G_r^k(m_S, n_S) \) satisfying Properties 1–5, and (II) we show how to construct such a function.

Proof of the statement. Take \( k \) to be a monotone function of \( d \) that satisfies \( \lim_{d \to \infty} k = \infty \) and \( k = O(d^{1/2}) \), where \( c \) is any constant such that \( 0 < c < 1 \). Thanks to Property 1 and Proposition A1, we have the following conditions:

- \( \gamma_k = 1 \) and \( \gamma_{k,k} \geq 2 + \frac{r - 1}{k - r + 1} \)
- To achieve an approximation guarantee that is better than \( \alpha_k^{-1} \) requires \( \Omega(d^{(r+1)}) \) times function evaluation.

Since we can take \( r \) to be any fixed positive integer satisfying \( r \leq k = O(d^{1/2}) \), we see that \( \Omega(d^{(r+1)}) \) is not polynomial in \( d \). Furthermore, we have \( \gamma_{k,k} \to \infty \) \( 1/2 \) and \( \alpha_k^{-1} \to \infty \) \( 1 - e^{-1} \). Hence we obtain the statement.

Construction of \( G_k^r \). Given any positive integer \( \ell \leq k \), we define the following function \( H^\ell(m, n) \) for integers \( m \in [0, \ell] \) and \( n \in [0, d] \) that satisfy \( m \leq n \):

\[
H^\ell(m, n) := \begin{cases} \ell - \ell^{-1}(\ell - m)(1 - \frac{1}{\ell})^{n-m} & \text{if } n \leq k + \ell, \\ \ell^n & \text{otherwise.} \end{cases}
\]

Note that the function is non-negative and that we have

\[
H^\ell(0, 0) = 0 \quad \text{and} \quad H^\ell(0, n) = H^\ell(1, n) = \ell^{n} \left(1 - \frac{1}{\ell}\right)^n.
\]

Given any integers \( m_1, n_1, m_2, n_2 \) such that

\[
0 \leq m_1 \leq n_1, \quad 0 \leq m_2 \leq n_2, \quad m_1 + m_2 \leq \ell, \quad \text{and} \quad n_1 + n_2 \leq d,
\]

we define

\[
H^\ell(m_2, n_2 | m_1, n_1) := H^\ell(m_1 + m_2, n_1 + n_2) - H^\ell-r+1(m_1, n_1) = \ell^{n_1 - m_1} \left(1 - \frac{1}{\ell}\right)^{n_2 - m_2} \left(\ell - m_1 - (\ell - m_1 - m_2) \left(1 - \frac{1}{\ell}\right)^{n_2 - m_2}\right).
\]

When \( (m_2, n_2) = (0, 1) \) and \( (1, 1) \), for any \( m_1, n_1 \) satisfying the above conditions, we have

\[
H^\ell(0, 1 | m_1, n_1) = \ell^{-1} \left(1 - \frac{m_1}{\ell}\right) \left(1 - \frac{1}{\ell}\right)^{n_1 - m_1} \quad \text{and} \quad H^\ell(1, 1 | m_1, n_1) = \ell^{-1} \left(1 - \frac{1}{\ell}\right)^{n_1 - m_1},
\]

respectively. For later use, we prove the following lemma:

Lemma A1. For any integers \( m_1, n_1, m_2, n_2 \) that satisfy

\[
0 \leq m_1 \leq n_1 \leq \ell, \quad 0 \leq m_2 \leq n_2 \leq k, \quad m_1 + m_2 \leq \ell, \quad \text{and} \quad n_1 + n_2 \leq d, \tag{A2}
\]

we have

\[
\frac{H^\ell(m_2, n_2 | m_1, n_1)}{m_2 H^\ell(0, 1 | m_1, n_1) + (n_2 - m_2) H^\ell(1, 1 | m_1, n_1)} \geq \left(2 + \frac{k - \ell}{\ell}\right)^{-1},
\]

where we regard \( 0/0 = 1 \).
Proof. We rewrite the LHS of the target inequality as follows:

\[
\frac{H^\ell(m_2, n_2 \mid m_1, n_1)}{m_2 H^\ell(0, 1 \mid m_1, n_1) + (n_2 - m_2) H^\ell(1, 1 \mid m_1, n_1)} = \frac{(1 - \frac{k}{\ell})^{n_1 - m_1} + (\frac{1}{\ell})^{n_1 - m_1} \left(1 - \frac{k}{\ell}\right)^{n_2 - m_2}}{m_2 \times (1 - \frac{k}{\ell})^{n_1 - m_1} + (\frac{1}{\ell})^{n_1 - m_1} \left(1 - \frac{k}{\ell}\right)^{n_2 - m_2}}
\]

By defining \(x := \frac{m_2}{\ell}, y := \frac{n_2}{\ell}\), and \(z := 1 - \frac{m_1}{\ell}\), we obtain

\[
\frac{H^\ell(m_2, n_2 \mid m_1, n_1)}{m_2 H^\ell(0, 1 \mid m_1, n_1) + (n_2 - m_2) H^\ell(1, 1 \mid m_1, n_1)} = \frac{z - (z - x) \left(1 - \frac{k}{\ell}\right)^{(y - x)}}{x(1 - z) + yz},
\]

where \(x, y, z\) must satisfy the following inequalities from (A2):

\[
0 \leq z \leq 1, \quad 0 \leq x \leq y \leq 1 + \frac{k - \ell}{\ell}, \quad x \leq z, \quad \text{and} \quad y - z \leq \frac{d}{\ell} - 1.
\]

The value of (A3) can be bounded from below by \(2 + \frac{k - \ell}{\ell}\) as follows:

\[
\frac{z - (z - x) \left(1 - \frac{k}{\ell}\right)^{(y - x)}}{x(1 - z) + yz} \geq \frac{z - (z - x) e^{-(y - x)}}{x(1 - z) + yz} \geq \frac{z - (z - x) \frac{1}{1 + y - x}}{x(1 - z) + yz} \geq \frac{1}{1 + y - x} \geq \left(2 + \frac{k - \ell}{\ell}\right)^{-1}. \quad \therefore \text{for } a > -1 \text{ we have } e^{-a} \leq \frac{1}{1 + a}
\]

Thus, the lemma holds. □

By using function \(H^\ell(m, n)\) defined above, we construct \(G^k_r(m, n)\) for any integers \(m \in [0, k]\) and \(n \in [0, d]\) as follows:

\[
G^k_r(m, n) := \begin{cases} 
2 \times H^{k-r+1}(0, 1) & \text{if } 0 \leq m \leq n \leq r, \\
(r - 1) H^{k-r+1}(0, 1) + H^{k-r+1}(0, n - r + 1) & \text{if } 0 \leq m \leq r \text{ and } r \leq n \leq d, \\
(r - 1) H^{k-r+1}(0, 1) + H^{k-r+1}(m - r + 1, n - r + 1) & \text{if } r \leq m \leq n \text{ and } r \leq n \leq d.
\end{cases}
\]

By using \(G^k_r\), we define \(F(S) = G^k_r(m_S, n_S)\). The function is defined in almost the same way as that in (28), and so we can confirm that \(G^k_r\) has Properties 2–5 in a similar manner. Below we show that the function has Property 1. The monotonicity can be confirmed easily by examining \(F(j \mid S)\) for each case. Furthermore, by analogy with the proof in (28), we can show that \(F(S) = G^k_r(m_S, n_S)\) is submodular over all subsets of size at most 2k: i.e., \(F(j \mid S) \geq F(j \mid T)\) for any \(S \subseteq T\) satisfying \(|T| < 2k\) and \(j \notin T\). This suffices to prove \(\gamma^k_k = 1\).

Below we prove \(\tilde{\gamma}^k_k \geq \left(2 + \frac{r - 1}{k - r + 1}\right)^{-1}\). Note that the supermodularity ratio can be written as

\[
\tilde{\gamma}^k_k = \min_{L, S : L \cap S = \emptyset, |L| \leq k, |S| \leq k} \frac{F(S \mid L)}{\sum_{j \in S} F(j \mid L)}.
\]

where we regard 0/0 = 1. In what follows, for any disjoint \(L, S \subseteq [d]\) of size at most \(k\), we consider bounding \(\sum_{j \in S} F(j \mid L)\) from below. Depending on the values of \(m_L = |L \cap M|, m_S = |S \cap M|, n_L = |L|,\) and \(n_S = |S|\), we have the following six cases. We first examine each case and then show that \(\sum_{j \in S} F(j \mid L) \geq \left(2 + \frac{r - 1}{k - r + 1}\right)^{-1}\) holds for all cases.
Case 1: \( n_S + n_L < r \). In this case, we have \( F(S \mid L) = (n_S - n_L)H^{k-r+1}(0,1) \); i.e., the function is modular. Therefore, we have \( \sum_{j \in S} F(j \mid L) = 1 \).

Case 2: \( n_L < r \) and \( m_L + m_S \leq r \leq n_S + n_L \). In this case, we have

\[
\begin{align*}
F(S \mid L) &= H^{k-r+1}(0,n_S + n_L - r + 1) - (n_L - r + 1)H^{k-r+1}(0,1), \\
F(j \mid L) &= H^{k-r+1}(0,1).
\end{align*}
\]

Due to the submodularity over all subsets of size at most \( 2k \), the more elements \( L \) includes, the smaller \( F(S \mid L) \) becomes, which means \( F(S \mid L) \) attains its minimum when \( n_L = r - 1 \). Therefore, we have

\[
\frac{F(S \mid L)}{\sum_{j \in S} F(j \mid L)} \geq \frac{H^{k-r+1}(m_S + m_L - r + 1, n_S)}{n_S \times H^{k-r+1}(0,1)} = \frac{H^{k-r+1}(m_S + m_L - r + 1, n_S \mid 0,0)}{n_S \times H^{k-r+1}(1,1 \mid 0,0)},
\]

where the last equality comes from \( H^{k-r+1}(0,n) = H^{k-r+1}(1,n) \).

Case 3: \( n_L < r \) and \( r \leq m_S + m_L \). We have

\[
\begin{align*}
F(S \mid L) &= H^{k-r+1}(m_L + m_S - r + 1, n_S + n_L - r + 1) - (n_L - r + 1)H^{k-r+1}(0,1), \\
F(j \mid L) &= H^{k-r+1}(0,1).
\end{align*}
\]

By analogy with the above case, \( F(S \mid L) \) attains its minimum when \( n_L = r - 1 \). Therefore,

\[
\frac{F(S \mid L)}{\sum_{j \in S} F(j \mid L)} \geq \frac{H^{k-r+1}(m_S + m_L - r + 1, n_S)}{n_S \times H^{k-r+1}(0,1)} = \frac{H^{k-r+1}(m_S + m_L - r + 1, n_S \mid 0,0)}{(m_S + m_L - r + 1)H^{k-r+1}(0,1 \mid 0,0) + (n_S - m_S - m_L + r - 1)H^{k-r+1}(1,1 \mid 0,0)},
\]

where the last equality comes from \( H^{k-r+1}(0,n) = H^{k-r+1}(1,n) \).

Case 4: \( m_L < r \leq n_L \) and \( m_S + m_L \leq r \). We have

\[
\begin{align*}
F(S \mid L) &= H^{k-r+1}(0,n_S + n_L - r + 1) - H^{k-r+1}(0,n_L - r + 1) \\
&= H^{k-r+1}(0,n_S \mid 0, n_L - r + 1), \\
F(j \mid L) &= H^{k-r+1}(0,1 \mid 0, n_L - r + 1),
\end{align*}
\]

and thus we obtain

\[
\frac{F(S \mid L)}{\sum_{j \in S} F(j \mid L)} = \frac{H^{k-r+1}(0,n_S \mid 0, n_L - r + 1)}{n_S \times H^{k-r+1}(1,1 \mid 0, n_L - r + 1)},
\]

where we used \( H^{k-r+1}(0,1 \mid 0, n) = H^{k-r+1}(0,n+1) - H^{k-r+1}(0,n) = H^{k-r+1}(1,n+1) - H^{k-r+1}(0,n) = H^{k-r+1}(1,1 \mid 0, n) \).

Case 5: \( m_L < r \leq n_L \) and \( m_S + m_L \geq r \). We have

\[
\begin{align*}
F(S \mid L) &= H^{k-r+1}(m_S + m_L - r + 1, n_S + n_L - r + 1) - H^{k-r+1}(0,n_L - r + 1) \\
&= H^{k-r+1}(m_S + m_L - r + 1, n_S \mid 0, n_L - r + 1), \\
F(j \mid L) &= H^{k-r+1}(0,1 \mid 0, n_L - r + 1),
\end{align*}
\]

and thus we obtain

\[
\frac{F(S \mid L)}{\sum_{j \in S} F(j \mid L)} = \frac{H^{k-r+1}(m_S + m_L - r + 1, n_S \mid 0, n_L - r + 1)}{n_S \times H^{k-r+1}(0,1 \mid 0, n_L - r + 1)} = \frac{H^{k-r+1}(m_S + m_L - r + 1, n_S \mid 0, n_L - r + 1)}{(m_S + m_L - r + 1)H^{k-r+1}(0,1 \mid 0, n_L - r + 1) + (n_S - m_S - m_L + r - 1)H^{k-r+1}(1,1 \mid 0, n_L - r + 1)},
\]

where we used \( H^{k-r+1}(0,1 \mid 0, n) = H^{k-r+1}(1,1 \mid 0, n) \).
Case 6: $m_L \geq r$. We have

$$F(S \mid L) = H^{k-r+1}(m_S + m_L - r + 1, n_S + n_L - r + 1) - H^{k-r+1}(m_L - r + 1, n_L - r + 1)$$

$$= H^{k-r+1}(m_S, n_S \mid m_L - r + 1, n_L - r + 1),$$

and thus we obtain

$$F(S \mid L) = \frac{H^{k-r+1}(m_S, n_S \mid m_L - r + 1, n_L - r + 1)}{\sum_{j \in S} F(j \mid L)}$$

In all cases, the value of $\frac{F(S \mid L)}{\sum_{j \in S} F(j \mid L)}$ is lower-bounded by $\left(2 + \frac{r-1}{r-k+1}\right)^{-1}$ thanks to Lemma A1 with $\ell = k - r + 1$. Note that $m_1, n_1, m_2, n_2$ in Lemma A1 do not always correspond to $m_L - r + 1, n_L - r + 1, m_S, n_S$, respectively. For example, in Case 5, we let

$$m_1 = 0, \quad n_1 = n_L - r + 1, \quad m_2 = m_S + m_L - r + 1, \quad \text{and} \quad n_2 = n_S,$$

which satisfy the conditions required in the lemma.

\section{Randomized FPT Approximation Algorithm}

\begin{algorithm}[h]
\caption{Rand-FPT-Approx}
1: Execute SingleRun() $T$ times and return the best solution.
2: \textbf{function} SingleRun()
3: \quad $S_0 \leftarrow \emptyset$
4: \quad \textbf{for} $i = 1, \ldots, k$ \textbf{do}
5: \quad \quad Choose $j \in [d] \setminus S_{i-1}$ randomly with probability proportional to $F(j \mid S_{i-1})$.
6: \quad $S_i \leftarrow S_{i-1} \cup \{j\}$.
7: \quad \textbf{return} $S_k$
\end{algorithm}

In this section, we prove the guarantee of Rand-FPT-Approx for weakly modular maximization. This is an extension of the result in [31] that considers an FPT algorithm for a subclass of monotone submodular maximization.

We first prove a key lemma, which provides a lower bound of the probability that $j \in S^*$ is chosen in each iteration of SingleRun().

\textbf{Lemma A2}. For $i \in [k]$, let $S_{i-1}$ be the partial solution that is constructed in the loops of SingleRun(). Then the probability $p \in [0, 1]$ that newly chosen $j \in [d] \setminus S_{i-1}$ is included in $S^*$ is bounded from below as follows:

$$p \geq \gamma_{k,k} \cdot \frac{F(S^* \mid S_{i-1})}{F([d] \mid S_{i-1})}.$$

\textbf{Proof}. The proof is obtained directly from the definitions of the submodularity and supermodularity ratios as follows:

$$p = \frac{\sum_{j \in S^* \setminus S_{i-1}} F(j \mid S_{i-1})}{\sum_{j \in [d] \setminus S_{i-1}} F(j \mid S_{i-1})} \geq \gamma_{S_{i-1}, S^* \setminus S_{i-1}} \cdot \frac{F(S^* \mid S_{i-1})}{F([d] \mid S_{i-1})} \geq \gamma_{k,k} \cdot \frac{F(S^* \mid S_{i-1})}{F([d] \mid S_{i-1})}.$$

Using this lemma we obtain the theorem as follows:

\textbf{Theorem 2}. Assume that $F$ is $(\gamma_{k,k}, \gamma_{k,d})$-weakly modular. Let $S^*$ be an optimal solution. For any $\epsilon > 0$, if Algorithm runs with $T \geq \left(\frac{1}{\gamma_{k,k,d}} \cdot \left(1 + \epsilon \right)^k \log \delta^{-1}\right)$, then the obtained solution $S$ satisfies $F(S) \geq (1 + \epsilon)F(S^*) - \epsilon F([d])$ with a probability of at least $1 - \delta$. 

18
We here prove the theoretical guarantees of the multi-stage algorithms. We suppose that the surrogate function,

\[ F([d]) - F(S_{i-1}) \leq (1 + \epsilon)(F([d]) - F(S^*)) \]  
\[ F([d]) - F(S_{i-1}) > (1 + \epsilon)(F([d]) - F(S^*)) \]  

(4A)  
(4B)

Once (4A) occurs for some \( i \in [k] \), then we have \( F(S_k) \geq F(S_{i-1}) \geq (1+\epsilon)F(S^*) - \epsilon F([d]) \) thanks to the monotonicity of \( F(\cdot) \). If (4B) occurs, we have

\[ \frac{F(S^*) - F(S_{i-1})}{F([d]) - F(S_{i-1})} \geq \frac{\epsilon}{1+\epsilon}. \]

Hence, newly chosen \( j \in [d] \backslash S_{i-1} \) is included in \( S^* \) with probability \( p \geq \gamma_k, k, d \cdot \frac{1}{1+\epsilon} \) thanks to Lemma A2; if this occurs \( k \) times, we have \( F(S_k) = F(S^*) \geq (1 + \epsilon)F(S^*) - \epsilon F([d]) \). Consequently, \texttt{SingleRun()} returns \( S_k \) that satisfies \( F(S_k) \geq (1 + \epsilon)F(S^*) - \epsilon F([d]) \) with a probability of at least \( q := \left( \gamma_k, k, d \cdot \frac{1}{1+\epsilon} \right)^k \). Therefore, setting \( T \geq \left[ \left( \frac{1}{\gamma_k, k, d} \cdot \frac{1}{1+\epsilon} \right)^k \log \delta^{-1} \right] = \left\lceil \frac{\log \delta^{-1}}{q} \right\rceil \), Algorithm \texttt{MultiRun()} finds a solution \( S \) such that \( F(S) \geq (1 + \epsilon)F(S^*) - \epsilon F([d]) \) with a probability of at least

\[ 1 - (1 - q)^T \geq 1 - (1 - q)^{\frac{\log \delta}{q}} \geq 1 - e^{\log \delta} = 1 - \delta. \]

Thus, the proof is completed.

\[ \square \]

### E Multi-stage Algorithms

**Algorithm 2** Multi-stage algorithm

1. \( U \leftarrow [d], S \leftarrow \emptyset \)
2. for \( i = 1, \ldots, m \) do
   3. \( B_i \leftarrow \text{argmax}_{B_{\subseteq U} \mid |B| \leq b_i} G_S(B) \)
4. \( S \leftarrow S \cup B_i \)
5. \( U \leftarrow U \setminus B_i \)
6. return \( S \)

We here prove the theoretical guarantees of the multi-stage algorithms. We suppose that the surrogate function, \( G_S(\cdot) \), is monotone, which means we have \( |B_i| = b_i \) in each \( i \)-th iteration. Let \( S_i = B_1 \cup \cdots \cup B_i \) for \( i \in [m] \) and \( S_0 = \emptyset \). We take \( S^* \) and \( x^* \), which satisfy \( k^* = |S^*| = ||x^*||_0 \), to be target solutions for weakly modular maximization and \( \ell_0 \)-constrained minimization, respectively. We first show the following lemma for later use:

**Lemma A3.** Given any \( \beta_1, \ldots, \beta_m \) such that \( \beta_i \in [0, 1] \ (i \in [m]) \), if we can find \( B_i \subseteq [d] \) such that \( b_i = |B_i| \leq k^* \) and

\[ F(B_i \mid S_{i-1}) \geq \beta_i \frac{b_i}{k^*} (F(S^*) - F(S_{i-1})) \]  

(A6)

in each \( i \)-th iteration \( (i \in [m]) \), then the following inequality holds:

\[ F(S_m) \geq \left( 1 - \exp \left( -\frac{1}{k^*} \sum_{i=1}^{m} \beta_i b_i \right) \right) F(S^*). \]

**Proof.** We first prove

\[ F(S_m) \geq \left( 1 - \prod_{i=1}^{m} \left( 1 - \beta_i \frac{b_i}{k^*} \right) \right) F(S^*) \]

(A7)

by induction on \( i = 1, \ldots, m \). If \( i = 1 \), the inequality holds due to (A6). Assume that we have

\[ F(S_{i-1}) \geq \left( 1 - \prod_{i' = 1}^{i-1} \left( 1 - \beta_{i'} \frac{b_{i'}}{k^*} \right) \right) F(S^*). \]

(A8)
Then we obtain
\[
F(S_i) \geq \beta_i \frac{b_i}{k^i} (F(S^*) - F(S_{i-1})) + F(S_{i-1}) \quad \vdash \text{(A6)}
\]
\[
\geq \beta_i \frac{b_i}{k^i} F(S^*) + \left(1 - \beta_i \frac{b_i}{k^i}\right) \left(1 - \prod_{i' = 1}^{i-1} \left(1 - \beta_i' \frac{b_i'}{k^i'}\right)\right) F(S^*) \quad \vdash \text{(A8)}
\]
\[
\geq \left(1 - \prod_{i' = 1}^{i} \left(1 - \beta_i' \frac{b_i'}{k^i'}\right)\right) F(S^*).
\]

Therefore, the above inequality holds for any \( i \in [m] \) by induction. By setting \( i = m \), we obtain \text{(A7)}.

As in [28], given a finite number of non-negative scalars, their geometric mean always bounds from below their arithmetic mean. Therefore, given any integer \( m > 0 \) and \( x_i \in [0, 1] \), we have
\[
\prod_{i=1}^{m} (1 - x_i) \leq \left(1 - \frac{1}{m} \sum_{i=1}^{m} x_i\right)^m \leq \exp \left(-\sum_{i=1}^{m} x_i\right).
\]

From \text{(A7)} and the above inequality with \( x_i = \beta_i \frac{b_i}{k^i} \), we obtain the lemma.

Thanks to the above lemma, we can prove the guarantees of \text{Multi-Greedy} and \text{Multi-OMP}.

**Theorem 3.** Let \( b_{\min}, b_{\max} \) be integers such that \( 0 < b_{\min} \leq b_{\max} \leq k^* \). Set \( b_1, \ldots, b_m \) so as to satisfy \( b_i \in [b_{\min}, b_{\max}] \) for \( i \in [m] \) and \( \sum_{i \in [m]} b_i = k \). If \( F \) is \((\gamma_{S_{\min}}, k^*, \gamma_{S_{\max}})\)-weakly modular, solution \( S_m \) obtained with \text{Multi-Greedy} satisfies
\[
F(S_m) \geq \left(1 - \exp \left(-\frac{1}{k^*} \sum_{i=1}^{m} \gamma_{S_{i-1}, k^*} \gamma_{S_{i-1}, b_i}\right)\right) F(S^*)
\]
\[
\geq \left(1 - \exp \left(-\gamma_{S_{\min}, k^*} \gamma_{S_{\max}} \frac{k}{k^*}\right)\right) F(S^*).
\]

**Proof.** To prove the theorem, it suffices that \( B_i \) chosen by \text{Multi-Greedy} in each iteration satisfies \text{(A6)} with \( \beta_i = \gamma_{S_{i-1}, k^*} \gamma_{S_{i-1}, b_i} \); then we can obtain the theorem by using Lemma\text{(A3)}. Note that \text{Multi-Greedy} uses \( G_{S_{i-1}}(B) = \sum_{j \in B} F(j \mid S_{i-1}) \) as a surrogate function in each \( i \)-th iteration. From \( b_i \leq k^* = |S^*| \) and the greedy rule, we have
\[
\frac{1}{b_i} \sum_{j \in B_i} F(j \mid S_{i-1}) \geq \frac{1}{k^*} \sum_{j \in S^* \setminus S_{i-1}} F(j \mid S_{i-1}). \quad \text{(A9)}
\]

Therefore, we obtain
\[
F(B_i \mid S_{i-1}) \geq \gamma_{S_{i-1}, b_i} \frac{b_i}{k^i} \sum_{j \in B_i} F(j \mid S_{i-1}) \quad \vdash \text{definition of } \gamma_{S_{i-1}, b_i}
\]
\[
\geq \gamma_{S_{i-1}, b_i} \frac{b_i}{k^i} \sum_{j \in S^* \setminus S_{i-1}} F(j \mid S_{i-1}) \quad \vdash \text{(A9)}
\]
\[
\geq \gamma_{S_{i-1}, k^*} \gamma_{S_{i-1}, b_i} \frac{b_i}{k^i} F(S^* \mid S_{i-1}) \quad \vdash \gamma_{S_{i-1}, k^*} \gamma_{S_{i-1}, b_i} \geq \gamma_{S_{i-1}, k^*} \quad \text{and } F(S^* \mid S_{i-1}) = F(S^* \mid S_{i-1})
\]
\[
\geq \gamma_{S_{i-1}, k^*} \gamma_{S_{i-1}, b_i} \frac{b_i}{k^i} (F(S^*) - F(S_{i-1})). \quad \vdash \text{monotonicity}
\]

Thus the proof is completed.

**Theorem 4.** Suppose that \( F \) is defined as \( F(S) = l(0) - \min_{\supp(x^*) \subseteq \supp(l)(x^*)} l(x^*) \) and \( b_1, \ldots, b_m \) are set as in Theorem \text{3}. Assume that \( l(\cdot) \) is \( \mu_{k+k^*} - \text{RSC} \) and \( \nu_{k,b_{\max}} - \text{RSM} \). If \( S_m \) is a solution obtained with \text{Multi-OMP}, then we have
\[
F(S_m) \geq \left(1 - \exp \left(-\frac{1}{k^*} \sum_{i=1}^{m} \frac{\mu_{S_{i-1}, S_{i-1} \cup S^*}}{\nu_{S_{i-1}, S_{i-1}} b_i}\right)\right) F(S^*)
\]
Consequently, solution $x = \arg\min_{\supp(x') \subseteq S_m} l(x')$ satisfies

$$l(x) \leq l(x^*) + \exp\left(-\frac{\mu k \cdot k^*}{\nu_{k,b_{\max}}} \right)(l(0) - l(x^*))$$

$$\leq l(x^*) + \exp\left(-\frac{1}{\nu_{k,b_{\max}}} \right)(l(0) - l(x^*)) .$$

**Proof.** As in Section 2, we define $f(x) := l(0) - l(x)$ and $b^{(S)} := \arg\max_{\supp(x) \subseteq S} f(x)$ for any given $S \subseteq [d]$. Analogous with the proof of Theorem 3, our aim is to prove (A6) with $\beta_i = \frac{\mu_{S_{i-1} \cup S^*}}{\nu_{S_{i-1} \cup S^*}}$. Note that Multi-OMP uses $G_{S_{i-1}}(B) = \sum_{j \in B} \|\nabla l(b^{(S_{i-1})})_j\|^2 = \sum_{j \in B} \|\nabla f(b^{(S_{i-1})})_j\|^2 = \|\nabla f(b^{(S_{i-1})})_B\|^2$ as a surrogate function. Therefore, by using $b_i \leq k^* = |S^*|$, $\nabla f(b^{(S_{i-1})})_{S_{i-1}} = 0$, and the greedy rule, we obtain

$$\frac{1}{b_i} \|\nabla f(b^{(S_{i-1})})_B\|^2 \geq \frac{1}{k} \|\nabla f(b^{(S_{i-1})})_{S^* \setminus S_{i-1}}\|^2. \quad (A10)$$

By using this inequality and Lemma 1, we obtain

$$F(B_i \mid S_{i-1}) \geq \frac{1}{2 \nu_{S_{i-1} \cup S^*}} \|\nabla f(b^{(S_{i-1})})_{B_i}\|^2$$

$$\geq \frac{1}{2 \nu_{S_{i-1} \cup S^*}} \cdot \frac{b_i}{k} \|\nabla f(b^{(S_{i-1})})_{S^* \setminus S_{i-1}}\|^2$$

$$\geq \frac{\mu_{S_{i-1} \cup S^*}}{\nu_{S_{i-1} \cup S^*}} \cdot \frac{b_i}{k} \|\nabla f(b^{(S_{i-1})})_{S^* \setminus S_{i-1}}\|^2$$

$$\geq \frac{\mu_{S_{i-1} \cup S^*}}{\nu_{S_{i-1} \cup S^*}} \cdot \frac{b_i}{k} (F(S^* \setminus S_{i-1} \mid S_{i-1}) - F(S_{i-1})).$$

Thus the theorem holds thanks to Lemma A3.