Scalable Greedy Feature Selection via Weak Submodularity

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Abstract

Greedy algorithms are widely used for problems in machine learning such as feature selection and set function optimization. Unfortunately, for large datasets, the running time of even greedy algorithms can be quite high. This is because for each greedy step we need to re-fit a model or calculate a function using the previously selected choices and the new candidate.

Two algorithms that are faster approximations to the greedy forward selection were introduced recently [Mirzasoleiman et al., 2013, 2015]. They achieve better performance by exploiting distributed computation and stochastic evaluation respectively. Both algorithms have provable performance guarantees for submodular functions.

In this paper we show that divergent from previously held opinion, submodularity is not required to obtain approximation guarantees for these two algorithms. Specifically, we show that a generalized concept of weak submodularity suffices to give multiplicative approximation guarantees. Our result extends the applicability of these algorithms to a larger class of functions. Furthermore, we show that a bounded submodularity ratio can be used to provide data dependent bounds that can sometimes be tighter also for submodular functions. We empirically validate our work by showing superior performance of fast greedy approximations versus several established baselines on artificial and real datasets.

1 Introduction

Consider the problem of sparse linear regression:

$$\min_{\beta} \|y - X\beta\|_2^2 \quad \text{s.t.} \quad \|\beta\|_0 \leq k,$$  \hspace{1cm} (1)

where $X \in \mathbb{R}^{n \times d}$ is the design matrix (also called feature matrix) for $n$ samples and $d$ features and $y \in \mathbb{R}^n$ is the corresponding vector of $n$ responses or observations. We assume without loss of generality that the columns of the matrix $X$ are normalized to 1, and the response vector is also normalized.

Given a subset $S$ of features (denoted by $X_S$), it is easy to find the best regression coefficients by projecting $y$ on the span of $X_S$. The $R^2$ statistic (coefficient of determination) measures the proportion of the variance explained by this subset. Sparse regression can be therefore seen as maximizing a set function $R^2(S)$: for any given set of columns $S$, $R^2(S)$ measures how well these columns explain the observations $y$.

This set function $R^2(S)$ is monotone increasing: including more features can only increase the explained variance. Solving sparsity constrained maximization of $R^2$ would involve searching over all subsets of size up to $k$ and selecting the one that maximizes $R^2$. This combinatorial optimization problem is unfortunately NP-Hard [Das and Kempe, 2011]. A widely used approach is to use greedy forward selection: select one feature at a time, greedily choosing the one that maximizes $R^2$. In the next step. Orthogonal Matching Pursuit and variations [Tropp, 2004] [Needell and Tropp, 2008] can also be seen as approximate accelerated greedy forward selection algorithms that avoid re-fitting the model for each candidate vector at each step.

When maximizing set functions using the greedy algorithm it is natural to consider the framework of submodularity. In a classical result, [Nemhauser et al., 1978] show that for submodular monotone functions, the greedy $k$-sparse solution is within $(1 - \frac{1}{e})$ of the optimal $k$-sparse solution, i.e., greedy gives a constant multiplicative factor approximation guarantee. The concept of submodularity has led to several effective greedy solutions to problems such as sparse prediction [Koyejo et al., 2014], sparse factor analysis [Khanna et al., 2015], model interpretation [Kim et al., 2016], etc.

Unfortunately, it is easy to construct counterexamples to show that $R^2(S)$ is not submodular [Das and Kempe, 2011, Elenberg et al., 2016]. In their breakthrough paper [Das and Kempe, 2011] show that if the design matrix $X$ sat-

\[\text{However, adjusted } R^2 \text{ is not monotonic.}\]
Satisfies the Restricted Isometry Property (RIP), then the set function $R^2(S)$ satisfies a weakened form of submodularity. This weak form of submodularity is obtained by bounding a quantity called a submodularity ratio $\gamma$ defined subsequently. The authors further showed that a bounded submodularity ratio $\gamma$ is sufficient for Nemhauser’s proof to go through with a relaxed approximation constant (that depends on $\gamma$). Therefore, even weak submodularity implies a constant factor approximation for greedy and RIP implies weak submodularity.

The weak submodularity framework was recently extended beyond linear regression by [Elenberg et al., 2016] to concave functions (for example, likelihood functions of generalized linear models). This generalization of the RIP condition is called Restricted Strong Convexity (RSC) and the general result is that RSC implies weak submodularity for the set function obtained from the likelihood of the model restricted to subsets of features. This shows that greedy feature selection can obtain constant factor approximation guarantees in a very general setting, similar to results obtained by Lasso but without further statistical assumptions.

Running the greedy algorithm can be computationally expensive for large datasets. This is because for each greedy step we need to refit the model using the previously selected choices and the new candidate. This has led to the development of faster variants. For example, DistributedGreedy [Mirzasoleiman et al., 2013] distributes the computational effort across available machines, and StochasticGreedy [Mirzasoleiman et al., 2015] exploits a stochastic greedy step. Both algorithms have provable performance guarantees for submodular functions.

In this paper, we show that submodularity is not required to obtain approximation guarantees for these two algorithms and that a bounded submodularity ratio suffices. This extends the scope of these algorithms to significantly larger class of functions like sparse linear regression with RIP design matrices. Furthermore, as we shall discuss, submodularity ratio can be used to provide data dependent bounds. This implies that one can sometimes obtain tighter guarantees also for submodular functions.

Our contributions are as follows: (1) We analyze and obtain approximation guarantees for DistributedGreedy and StochasticGreedy using the submodularity ratio extending the scope of their application to non-submodular functions, (2) We show that the submodularity ratio can give tighter data dependent bounds even for submodular functions, (3) We derive explicit bounds for both DistributedGreedy and StochasticGreedy for the special case of sparse linear regression, (4) We derive bounds for sparse support selection for general concave functions, (5) We also present empirical evaluations of these algorithms vs several established baselines on simulated and real world datasets.

Related Work [Das and Kempe, 2011] defined submodularity ratio, and showed that for any function that has its submodularity ratio bounded away from 0, one can provide appropriate greedy guarantees. [Elenberg et al., 2016] used the concept to derive a new relationship between submodularity and convexity, specifically stating that the Restricted Strong Concavity can be used to bound the submodularity ratio. This results in providing bounds for greedy support selection for general concave functions.

Another notion of approximate additive submodularity was explored by [Krause and Cevher, 2010] for the problem of dictionary selection. This was, however, superseded by [Das and Kempe, 2011] who showed that submodularity ratio provides tighter approximation bounds. [Horel and Singer, 2016] consider another generalization from submodular functions – $\varepsilon$-approximate submodular functions which are functions within $\varepsilon$ of some submodular function, and provide approximation guarantees for greedy maximization.

The DistributedGreedy algorithm was introduced by [Mirzasoleiman et al., 2013]. They provide deterministic bounds for any arbitrary distribution of data onto the individual machines. [Barbosa et al., 2013] showed that for sparsity constraints, and under the assumption that the data is split uniformly at random to all the machines, one can obtain a $1/(1-e^{\varepsilon})$ guarantee in expectation. [Kumar et al., 2013] also provide distributed algorithms for maximizing a monotone submodular function subject to a sparsity constraint. They extend the Threshold Greedy algorithm of [Gupta et al., 2010] by augmenting it with a sample and prune strategy. It runs the Threshold Greedy algorithm on a subset of data to obtain a candidate solution. The latter is then used to prune the remaining data to reduce its size. This process is repeated a constant number of times, and the algorithm provides a constant factor guarantee.

[Bhaskara et al., 2016] provide approximation guarantees for greedy selection variants for column subset selection. They do not use the submodularity framework, and their results are not directly applicable or useful for other problem settings. Similarly, [Farahat et al., 2013] also use greedy column subset selection. However, their focus is not towards obtaining approximation guarantees, but rather on more efficient algorithmic implementation.

2 Background

Notation: We represent vectors as small letter bolds e.g. $u$. Matrices are represented by capital bolds e.g. $X, T$. Matrix or vector transposes are represented by superscript $X^\top$. Identity matrices of size $s$ are represented by $I_s$, or simply $I$ when the dimensions are obvious. $1(0)$ is a column vector of all ones (zeroes). Sets are represented by sans serif fonts.
The submodularity ratio of a set

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Definition 1 (Submodularity Ratio [Das and Kempe 2011]). Let $S, L \subset [d]$ be two disjoint sets, and $f : [d] \rightarrow \mathbb{R}$. The submodularity ratio for $S$ with respect to $L$ is given by

$$
\gamma_{LS} := \frac{\sum_{j \in S} [f(L \cup \{j\}) - f(L)]}{f(L \cup S) - f(L)}.
$$

The submodularity ratio of a set $U$ with respect to an integer

$k$ is given by

$$
\gamma_{U,k} := \min_{L : S \subseteq L, \gamma_{LS} > 0, L \subseteq U, |S| \leq k} \gamma_{LS}.
$$

It is straightforward to show that $f$ is submodular if and

only if $\gamma_{LS} \geq 1$ for all sets $L$ and $S$. Generalizing to the functions with $0 < \gamma_{LS} \leq 1$ provides a notion of weak submodularity [Elenberg et al. 2016]. For weakly submodular functions, even though the function may not be submodular, it still provides approximation guarantees for the greedy algorithm. We use the submodularity ra-

tio to provide new bounds for DISTRIBUTEDGREEDY and STOCHASTICGREEDY, thereby generalizing these algo-

rithms to non-submodular functions.

2.1 Greedy Selection

We briefly go over the classic greedy algorithm for subset

selection. A greedy approach to optimizing a set function is myopic – the algorithm chooses the element from the available choices that gives the largest incremental gain for the set of choices previously made. The algorithm is illustrated in Algorithm 1. The algorithm makes $k$ outer iterations, where $k$ is the desired sparsity. Each iteration is a full pass over the remaining candidate choices, wherein the marginal gain is calculated for each remaining candidate choice. Thus the greedy algorithm has the computational complexity of $O(dk)$ calls to the function evaluation oracle.

For a large $d$, the linear scaling of the greedy algorithm for a fixed $k$ may be prohibitive. As such, algorithms that scale sublinearly are useful for truly large scale selections. The DISTRIBUTEDGREEDY algorithm, for example, achieves

this sublinear scaling by making use of multiple machines. The data is split uniformly at random to $l$ machines. Each

machine then performs its own independent greedy selection (Algorithm 1), and outputs a $k$ sized solution. All of the greedy solutions are collated by a central machine, which performs another round of the greedy selections to output the final solution. The algorithm is illustrated in Algorithm 2, and is analyzed in Section 3. It has a computational complexity of $O(dk/l)$! The algorithm is easy to implement in parallel or within a distributed computing framework e.g. MapReduce.

Algorithm 1 GREEDY$(S, k)$

1: Input: sparsity $k$, available choices $S$
2: $A_0 = \emptyset$
3: for $i \in 0 \ldots (k - 1)$ do
4:     $s = \arg \max_{j \in S \setminus A_i} f(A_i \cup \{j\}) - f(A_i)$
5:     $A_{i+1} = A_i \cup \{s\}$
6: end for
7: return $A_k$

An alternative to distributing the data, say when several machines are not available, is to perform the greedy selection stochastically. The STOCHASTICGREEDY algorithm for submodular functions was introduced by [Mirzasoleiman et al. 2015]. At any given iteration $i \in [k]$, instead of performing a function evaluation for each of the remaining $(d - i)$ candidates, a subset of a fixed size $C = \lceil d \log \frac{l}{\delta} \rceil$ (where $\delta$ is a pre-specified hyperparameter) is uniformly sampled from the available $(d - i)$ choices using the subroutine SUBSAMPLE, and the function evaluation is made on those subsampled choices as if they were the only available candidates. This speeds up the greedy algorithm to $O(Ck)$ function evaluations. The algorithm is presented in Algorithm 3, and its approximation bounds are discussed in Section 4.

Algorithm 2 DISTRIBUTEDGREEDY$(l, k, \{A_j\})$

1: Input: sparsity $k$, number of parallel solvers $l$, partition \{A_j\} of the set of available choices $A$
2: $G_i \leftarrow \text{GREEDY}(A_j, k) \forall j \in [l]$
3: $G \leftarrow \text{GREEDY} (\cup_j G_j, k)$
4: $G_{\text{max}} \leftarrow \arg \max_{G} f(G)$
5: return $\arg \max_{G} f(G), f(G_{\text{max}})$

Finally, we discuss a property of the greedy algorithm, which is fundamental to the analysis of the DISTRIBUTEDGREEDY algorithm. The greedy algorithm belongs to a larger class of algorithms called 1-nice algorithms [Mirrokhni and Zadimoghaddam 2015]. The following result allows us to remove or add unselected items from the choice set that is accessible to the algorithm.

Lemma 1. [Mirrokhni and Zadimoghaddam 2015] Say $|S| > k$, and let GREEDY$(S, k) \subset S$ be the $k$-sized set
Algorithm 3 StochasticGreedy(S, k, δ)

1: Input: sparsity k, available choices S, subsampling parameter δ
2: A0 = ∅
3: for i ∈ 0 . . . (k − 1) do
4:     Sδ ← Sample(S \ Aδ, δ, k)
5:     s = arg maxj∈S f(Ai ∪ {j}) − f(Ai)
6:     Ai+1 = Ai ∪ {s}
7: end for
8: return A

return by Algorithm [7] For any x /∈ Greedy(S, k), Greedy(S \ {x}, k) = Greedy(S, k).

Note that Lemma [1] is a property of the algorithm, and is independent of the function itself. Prior works [Mirrokni and Zadimoghaddam 2015, Barbosa et al. 2015] have exploited this property in conjunction with properties of submodular functions to obtain approximation bounds for the distributed algorithms. Our work extends these results to weakly submodular functions. As such, it is easy to see that our results are easily extensible to other nice algorithms – including distributed OMP and distributed stochastic greedy – that have closed form bounds for the respective single machine algorithm. For ease of exposition, we focus our discussion on the distributed greedy algorithm.

3 Distributed Greedy

In this section, we obtain approximation bounds for DistributedGreedy (Algorithm [2]). The algorithm returns the best out of (l + 1) solutions : the l local solutions (steps 2,4), and the final aggregated one (step 3). Our strategy to obtain the approximation bound for the algorithm is as follows. To obtain an overall approximation bound, we obtain individual bounds on each of the solutions in terms of the submodularity ratio (Definition [1]) and use the subadditivity ratio (Definition [2]) to show that one of the two shall always hold. For approximation bounds on the local solutions, we make use of the niceness of the Greedy (Lemma [1]). The bound on the aggregated solution is more involved, since it involves tracking the split of the true solution A* across machines. The assumption of partitioning uniformly at random is vital here. This helps us lower bound the greedy gain in expectation by a probabilistic overlap with the true solution. The trick of tracking the split of the true solution across machines is similar to the one that has been used for analysis of submodular functions [Mirrokni and Zadimoghaddam 2015, Barbosa et al. 2015], but without the explicit connection to submodularity and subadditivity ratios. As we shall see in Sections [5][6] elucidating these connections leads to novel bounds for support selection for linear regression and general concave functions.

We next define the subadditivity ratio, which helps us generalize subadditive functions in the way similar to how submodularity ratio generalizes submodular functions.

Definition 2 (Subadditivity ratio). We define the subadditivity ratio for a set function f w.r.t a set S as:

$$\nu_S := \min_{A \cup B = S} \frac{f(A) + f(B)}{f(S)}.$$ 

We further define the subadditivity ratio of a function for an integer k, $\nu_k$, which takes a uniform bound over all sets of size k:

$$\nu_k := \min_{S: |S| = k} \nu_S.$$ 

By definition, the function $f(\cdot)$ is subadditive iff $\nu_S \geq 1, \forall S \subset [d]$. Since submodularity implies subadditivity (the converse is not always true), if the function $f(\cdot)$ is submodular, $\nu_S \geq 1, \forall S \subset [d]$.

We next present some notation and few lemmas that lead up to the main result of this section (Theorem [1]). Let A be the entire set of available choices. Partition the set A uniformly at random into A1, . . . , Ak. Let $G_j$ be the k-sized solution returned by running the greedy algorithm on Aj i.e. $G_j = Greedy(A_j, k)$. Note that each A induces a partition onto the optimal k-sized solution A* as follows:

$$S_j := \{x \in A^* : x \in Greedy(A_j \cup x, k)\},$$

$$T_j := \{x \in A^* : x \notin Greedy(A_j \cup x, k)\}.$$ 

Having defined the notation, we start by lower bounding the local solutions in terms of value of the subset of A* that is not selected as part of the respective local solution.

Lemma 2. $f(G_j) \geq (1 - (\exp(-\gamma_{G_j, k})) f(T_j)$.

The next lemma is used to lower bound the value of the aggregated solution (step 4 in Algorithm [2]) in terms of the value of the subset A* that is selected as part of the respective local solution.

Lemma 3. $\exists j \in [l] s.t. E[f(G)] \geq (1 - \frac{1}{\nu_k}) f(S_j).$

We are now ready to present our main result about the approximation guarantee for Algorithm [2].

Theorem 1. Let $G_{d_j}$ be the set returned by the distributed greedy (Algorithm [2]). Let $\gamma = \min\{\gamma_{G, k}, \gamma_{G, k}\}$. Then,

$$E[f(G_{d_j})] \geq \frac{\nu_k}{2} \left(1 - (1 - \exp(-\gamma))\right) f(A^*).$$

Proof. There are l machines, each with its local greedy solution $G_i, i \in [l]$. In addition, there is the aggregated solution set G. The key idea is to show that at least one of the (l + 1) solutions is good enough.

Say $f(T_i) \geq \frac{\nu_k}{2} f(A^*)$ for some i, then by Lemma 2 $f(G_i) \geq \frac{\nu_k}{2}(1 - (1 - \exp(-\gamma_{G_i, k})) f(A^*)$. 

On the other hand, say for all $i$, $f(T_i) < \frac{\nu_k}{\delta} f(A^*)$, then for all $i$, $f(S_i) > \frac{\delta}{\nu_k} f(A^*)$. By Lemma 3 the result then follows.

Theorem 2 generalizes the approximation guarantee of $\frac{1}{2}(1 - \frac{1}{e})$ obtained by [Barbosa et al. 2015] for submodular functions. Their analysis uses convexity of the Lovasz extension of submodular functions, and hence cannot be trivially extended to weakly submodular functions. In addition to being applicable for a larger class of functions, our result can also provide tighter bounds for specific applications or datasets even for submodular functions, since they are also applicable for submodular functions, and bounding $\nu_k$ and $\gamma$ away from 1 from domain knowledge will give tighter approximations than the generic bound of $\frac{1}{2}(1 - \frac{1}{e})$.

4 Stochastic Greedy

For analysis of Algorithm 3 we show that the subsampling parameter $\delta$ governs the tradeoff between the speedup and the loss in approximation quality vis-a-vis the classic Greedy. Before formally providing the approximation bound, we present an auxiliary lemma that is key to proving the new approximation bound. The following result is a generalization of Lemma 2 from [Mirasoleiman et al. 2015] for weakly submodular functions.

Lemma 4. Let $A, B \subset [n]$, with $|B| \leq k$. Consider another set $C$ drawn randomly from $[n] \setminus A$ with $|C| = \lceil \frac{n \log \frac{1}{\delta}}{k} \rceil$. Then,

$$E[\max_{v \in C} f(v \cup A) - f(A)] \geq \frac{(1 - \delta)\gamma_{A,B\cup A}}{k} (f(B) - f(A)).$$

We are now ready to present our result that shows that stochastic greedy selections (Algorithm 3) can be applied to weakly submodular functions with provable approximation guarantees. All the proofs missing from the main text are presented in the supplement.

Theorem 2. Let $A^*$ be the optimum set of size $k$, and $A_i = \{a_1, a_2, \ldots, a_i\}, i \leq k$ be the set built by STOCHASTICGREEDY at step $i$. Then, $E[f(A_k)] \geq \left(1 - \frac{1}{e^{\gamma_{A^*,k}}} - \delta\right) f(A^*)$.

Proof. Define $g_i := f(A_i) - f(A_{i-1})$. Using Lemma 4 with $B = A^*$ and $\gamma_{A_{i-1},B\cup A} \geq \gamma_{A^*,k}$, we get at the $i$-th step,

$$E[g_i | A_{i-1} = A] \geq \frac{(1 - \delta)\gamma_{A^*,k}}{k} (f(B) - f(A)) \geq \frac{(1 - \delta)\gamma_{A^*,k}}{k} (f(A^*) - f(A)). \quad (6)$$

Define $h_{i-1} := E[f(A^*) - f(A_{i-1})]$, $C := \frac{(1 - \delta)\gamma_{A^*,k}}{k}$. Note that $E[g_i] = h_{i-1} - h_i$. Taking expectation on both sides over $A_i$, (6) becomes

$$h_i \leq (1 - C)h_{i-1} \leq (1 - C)^i h_0.$$

Using $h_k = E[f(A^*) - f(A_k)]$ and $h_0 = f(A^*)$ above, along with the fact that $1 + ad \geq a^d$ for $0 \leq \delta \leq 1$,

$$E[f(A_k)] \geq \left(1 - \left(1 - \frac{1}{e^{\gamma_{A^*,k}}} - \delta\right)^k\right) f(A^*) \geq \left(1 - \exp\left(-\gamma_{A^*,k} (1 - \delta)\right)\right) f(A^*) \geq \left(1 - \frac{1}{e^{\gamma_{A^*,k}}} - \delta\right) f(A^*).$$

Note that $\delta$ is the tradeoff hyperparameter between the speedup achieved by subsampling and the corresponding approximation guarantee. A larger value of $\delta$ means the algorithm is faster with weaker guarantees and vice versa. As $\delta \to 0$, we tend towards the bound $(1 - 1/e^{\gamma_{A^*,k}})$ which recovers the bound for weakly submodular functions obtained by [Das and Kempe 2011] for the classic greedy selections (Algorithm 1), and also recovers the well known bound of $(1 - 1/e)$ for submodular functions.

5 Large Scale Sparse Linear Regression

In this section, we derive novel bounds for greedy support selections for linear regression using both Algorithms 2 and 3. Recall that $X \in \mathbb{R}^{n \times d}$ is the feature matrix, with $n$ samples and $d$ features, and $y \in \mathbb{R}^n$ is the vector of $n$ responses. We assume, without loss of generality, that the columns of the matrix $X$ are normalized to 1, and the response vector is also normalized to have norm 1. Let $C \in \mathbb{R}^{d \times d}$ be the covariance matrix.

We know from standard linear algebra, that for a fixed set of columns $X_S$, where $S \subset [d]$ is the index into columns of $X$, $\beta_S^* = (X_S^T X_S)^{-1} X_S^T y$. Minimizing the error in (1) is thus equivalent to maximizing the following set function (modulo a constant $\|y\|_2^2$):

$$f(S) := \|P_Sy\|_2^2,$$

where $P_S := X_S(X_S^T X_S)^{-1} X_S^T$ is the projection matrix for orthogonal projection onto the span of columns of $X_S$. $f(\cdot)$ as defined above is also the $R^2$ statistic for the linear regression problem (1). The respective combinatorial maximization is:

$$\max_{|S| \leq k} f(S). \quad (8)$$

The function defined in (8) is not submodular. However, submodularity is not required for giving guarantees for
greedy forward selection. A bounded submodularity ratio is a weaker condition that is sufficient to provide such approximation guarantees. Das and Kempe [2011] analyzed the greedy algorithm for RSC, and showed that this function was weakly submodular. Our goal is to maximize the R² statistic for linear regression using Algorithms 2, 3.

For a positive semidefinite matrix C, \( \lambda_{\text{max}}(C, k) \) and \( \lambda_{\text{min}}(C, k) \) be the largest and smallest k-sparse eigenvalue of C. We make use of the following result from Das and Kempe [2011]:

**Lemma 5.** For the R² statistic in (7), \( \gamma_{S, k} \leq \lambda_{\text{max}}(C, k+|S|) \).

Recall that we need to only bound the submodularity ratio \( \gamma_{S, k} \) over the selected greedy set to obtain the approximation bounds (See Theorems 1 and 2). Lemma 5 provides a data dependent union bound for the submodularity ratio in terms of sparse eigenvalue of the covariance matrix. We now provide the corresponding approximation bounds for Algorithm 3 next.

**Corollary 1.** Let \( A^* \) be the optimal support set for sparsity constrained maximization of the R² statistic of convexity to submodularity to provide support selection guarantees. For a positive semidefinite matrix C, \( \lambda_{\text{max}}(C, k) \) and \( \lambda_{\text{min}}(C, k) \) be the largest and smallest k-sparse eigenvalue of C. We make use of the following result from Das and Kempe [2011]:

**Lemma 5.** For the R² statistic in (7), \( \gamma_{S, k} \leq \lambda_{\text{max}}(C, k+|S|) \).

Recall that we need to only bound the submodularity ratio \( \gamma_{S, k} \) over the selected greedy set to obtain the approximation bounds (See Theorems 1 and 2). Lemma 5 provides a data dependent union bound for the submodularity ratio in terms of sparse eigenvalue of the covariance matrix. We now provide the corresponding approximation bounds for Algorithm 3 next.

**Corollary 1.** Let \( A_{sg} \) be the optimal support set for sparsity constrained maximization of the R² statistic. Let \( A_{sg} \) be the solution returned by STOCHASTICGREEDY (S, k, δ). Then,

\[
\mathbb{E}[f(A_{sg})] \geq 1 - \frac{1}{1 - \frac{1}{\lambda_{\text{min}}(C, 2k)} - \delta} \cdot f(A^*).
\]

To obtain bounds for Algorithm 2, we also need to bound the subadditivity ratio (recall Definition 2).

**Lemma 6.** For the maximization of the R² statistic in (7), \( \nu_S \leq \frac{\lambda_{\text{max}}(C_S)}{\lambda_{\text{min}}(C_S)} \), where \( C_S \) is the submatrix of C with rows and columns indexed by S.

We can now provide the bounds for greedy support selection using Algorithm 2 for the linear regression problem.

**Theorem 3.** Let \( A_{sg} \) be the solution returned by the DISTRIBUTEDGREEDY algorithm, and let \( A^* \) be the optimal solution for the sparsity constrained maximization of R². Then,

\[
f(A_{sg}) \geq \frac{1}{2} \frac{\lambda_{\text{min}}(C_{A^*})}{\lambda_{\text{max}}(C_{A^*})} \left( 1 - \exp(-\frac{\lambda_{\text{min}}(C, 2k)}{\lambda_{\text{max}}(C, k)}) \right) f(A^*) \geq \frac{1}{2} \frac{\lambda_{\text{min}}(C, k)}{\lambda_{\text{max}}(C, k)} \left( 1 - \exp(-\frac{\lambda_{\text{min}}(C, 2k)}{\lambda_{\text{max}}(C, k)}) \right) f(A^*).
\]

**Proof.** Follows from Lemma 5 and by a uniform bound on \( \gamma \) in Theorem 1 as \( \gamma \geq \lambda_{\text{min}}(C, 2k) \) (from Lemma 5).

6 Support Selection for general functions

In this section, we leverage recent results from connections of convexity to submodularity to provide support selection bounds for Algorithms 2, 3 for general concave functions.

The sparsity constraint problem with a given \( k \leq d \) for a concave function \( g : \mathbb{R}^d \rightarrow \mathbb{R} \) is:

\[
\max_{|x|_0 \leq k} g(x). \tag{9}
\]

Similar to the developments in Section 5, we can define an associated set function as:

\[
f(S) := \max_{\supp(x) \subset S} g(x) - g(0). \tag{10}
\]

We recall that the submodular guarantee of \( g \) is for normalized submodular functions. To extend the notion of normalization to general support selection, we subtract \( g(0) \).

To bound the submodularity ratio for \( f(\cdot) \) in (10), the concept of strong concavity and smoothness is required. For a function \( g : \mathbb{R}^d \rightarrow \mathbb{R} \), define \( \mathcal{D}_g(x, y) := g(y) - g(x) - \langle \nabla g(x), y - x \rangle \). We say \( g(\cdot) \) is \( m \)- Restricted Strongly Convex (RSC) and \( L \)-Restricted Strongly Smooth (RSM) over a subdomain \( \Omega \subset \mathbb{R}^d \) if

\[
-m\Omega \| y - x \|_2^2 \geq \mathcal{D}_g(x, y) \geq -\frac{L}{4} \| y - x \|_2^2.
\]

We make use of the following result that lower bounds the submodularity ratio for \( f(\cdot) \):

**Lemma 7** (Elenberg et al. [2016]). If the given function \( g(\cdot) \) is \( m \)-strongly concave on all \( |S| + k \) sparse supports and \( L \)-smooth over all \( |S| + 1 \) sparse supports,

\[
\gamma_{S, k} \geq \frac{m}{L}.
\]

**Corollary 2.** Say the function \( g(x) : \mathbb{R}^d \rightarrow \mathbb{R} \) satisfies the assumptions of Lemma 7. Let \( A^* \) be the optimal support set that maximizes \( g(\cdot) \) under the sparsity constraint (9). Let \( A_{sg} \) be the solution set returned by STOCHASTICGREEDY. Then,

\[
\mathbb{E}[f(A_{sg})] \geq 1 - \frac{1}{1 - \frac{m}{L} - \delta} \cdot f(A^*).
\]

6.1 RSC implies Weak Subadditivity

In this section, we establish a lower bound on the subadditivity ratio in terms of only the restricted strong concavity (RSC) and smoothness (RSM) constants. This is analogous to lower bounding the submodularity ratio by Elenberg et al. [2016].

**Theorem 4.** Say the function \( g(x) : \mathbb{R}^d \rightarrow \mathbb{R} \) is \( m \) strongly concave and \( L \)-smooth over all \( x \supp \) supported on \( S \). Then, the subadditivity ratio can be lower bounded as:

\[
\nu_S \geq \frac{m}{L}. \tag{11}
\]
Proof. To prove Theorem 4 we make use of the following two results. Recall that for a set $S$ and vector $u$, $u_S$ denotes the subvector of $u$ supported on $S$.

Lemma 8. For a support set $S \subset [d]$, $f(S) \geq \frac{1}{2L} \|\nabla g(0)_S\|_F^2$.

Lemma 9. For any support set $S \subset [d]$, $f(S) \leq \frac{1}{2m} \|\nabla g(0)_S\|_F^2$.

Let $A, B$ be a partition of a given support set $S \subset [d]$ i.e $A \cup B = S, A \cap B = \emptyset$.

We can use Lemma 8 to lower bound the numerator of the subadditivity ratio as follows:

$$f(A) + f(B) \geq \frac{1}{2L} (\|\nabla g(0)_A\|_F^2 + \|\nabla g(0)_B\|_F^2)$$

Combining (12) with Lemma 9 we get,

$$\nu_S = \frac{f(A) + f(B)}{f(S)} \geq \frac{m}{L}.$$

Since we have a bound for the subadditivity ratio for general strongly concave and smooth functions, we can now provide a novel approximation guarantee for support selection by DistributedGreedy.

Corollary 3. Say the function $g(x) : \mathbb{R}^d \rightarrow \mathbb{R}$ is $m$-strongly concave over all $2k$ sparse support sets and $L$-smooth over all $k + 1$ sparse support sets. Let $A^*$ be the optimal support set that maximizes the sparsity constrained $g(\cdot)$ (9). Let $A_{dp}$ be the solution set returned by DistributedGreedy. Then,

$$\mathbb{E}[f(A_{dp})] \geq \frac{m}{2L} \left(1 - e^{-m/L}\right) f(A^*).$$

To the best of our knowledge, the bounds obtained in Corollary 3 are the first for a distributed algorithm for support selection for general functions. Note that we have taken a uniform bound for restricted strong concavity and smoothness to be over all $k$ sized support sets, though it is only required to be over the optimal support set.

7 Experiments

7.1 Distributed Linear Regression

We consider sparse linear regression in a distributed setting. We generate a 100-sparse regression vector is generated by selecting random nonzero entries of $\beta$,

$$\beta_s = (-1)^{\text{Bern}(1/2)} \times \left(5\sqrt{\frac{\log d}{n}} + \delta_s\right),$$

where $\delta_s$ is a standard i.i.d. Gaussian. Measurements $y$ are taken according to $y = X\beta + z$, where $\forall i \in [n], z_i$ is i.i.d. Gaussian with variance set to be $0.01\|X\beta\|_2^2$. Each row of the design matrix $X$ is generated by an autoregressive process,

$$X_{n,t+1} = \sqrt{1 - \alpha^2}X_{n,t} + \epsilon_{n,t},$$

where $\epsilon_{n,t}$ is i.i.d. Gaussian with variance $\alpha^2 = 0.25$. We take $n = 800$ for the number of both training and test measurements. Results are averaged over 10 iterations, each with a different partition $\{A_j\}$ of the 1000 features.

We evaluate four variants of DistributedGreedy. The two greedy algorithms are Greedy Forward Selection (FS) and Orthogonal Matching Pursuit (OMP). Lasso sweeps an $\ell_1$ regularization parameter $\lambda$ using LARS [Efron et al.].
Scalable Greedy Feature Selection via Weak Submodularity

Figure 2: Distributed linear regression, Electricity dataset.

This produces nested subsets of features corresponding to a sequence of thresholds for which the support size increases by 1. Lasso uses this threshold, while Lasso+ fits an unregularized linear regression on the support set selected by Lasso.

Figure 3 shows the performance of all algorithms on the following metrics: log likelihood (normalized with respect to a null model), generalization to new test measurements from the same true support parameter, area under ROC, and percentage of the true support recovered for $l = 10$.

Figure 3: Trade off in time vs log likelihood for various values of $\delta$-Stochastic Greedy as opposed to Greedy Forward Selection for logistic regression on gisette data [Lichman, 2013]. Results averaged over 10 iterations.

Next, we run a similar experiment on a large, real-world dataset. We sample $d = 140,250$ time series measurements across $n = 370$ customers from the ElectricityLoadDiagrams time series dataset [Lichman, 2013]. We consider the supervised learning experiment of predicting the electrical load at the next time 140,251. We use half of the customers for training and the rest for testing. Figure 4 shows performance of the same algorithms with data distributed across $l = 50$ partitions to select the top $k = 15$ features. We see that distributed Forward Selection produces both largest likelihood and highest generalization score. OMP has second largest likelihood, but its generalization varies widely for different values of $k$. This is likely due to the random placement of predictive features across a large number of partitions.

7.2 Stochastic Sparse Logistic Regression

In this section we demonstrate the applicability of Algorithm 5 for greedy support selection for sparse logistic regression. Note that the respective set function (10) when $g(\cdot)$ is the log likelihood for logistic regression is not submodular. As such one would not typically apply the STOCHASTICGREEDY algorithm for sparse logistic regression. However, the guarantees obtained in Section 6 suggest good practical performance which is indeed demonstrated in Figure 5. For the experiment we use the gisette dataset obtained from the UCI website [Lichman, 2013]. The dataset is of a handwritten digit recognition problem to separate out digits ‘4’ and ‘9’. It has 13500 instances, and 5000 features. Figure 3 illustrates depicts the tradeoff between the time taken to learn the model and the respective training log likelihood for different values of $\delta$ as used in Algorithm 3. As shown, we obtain tremendous speed up with relatively little loss in the log likelihood value even for reasonably large $\delta$ values.

8 Conclusion

We provided novel bounds for two greedy algorithm variants for maximizing weakly submodular functions with applications to linear regression and general concave functions. Our research opens questions on what other known algorithms with provable guarantees for submodular functions can be extended to weakly submodular functions.

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References

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A Proofs

In this section, we provide detailed proofs of all the results
used in this manuscript. For lemma and theorem statements
repeated from the main text, we add an apostrophe to indi-
cate that it is not a new lemma/theorem being introduced.

We make use of the following result that provides an ap-
proximation bound for greedy selections for weakly submodular
functions.

Lemma 10. [Das and Kempke 2011] Let \( S^* \) be the op-
timal \( k \)-sized set that maximizes \( f(\cdot) \) under the \( k \)-sparsity
constraint (see [2]). Let \( S_G \) be the set returned by greedy
forward selection (Algorithm 1), then

\[
E[f(B_{i+1}) - f(B_i)] \\
\geq \frac{1}{k} \sum_{x \in A^*} P(x \in \cup_{j \in [l]} G_j) E[f(x \cup B_i) - f(B_i)]
\]

\[
= \frac{1}{k} \sum_{j=1}^{l} \left( \sum_{x \in S_j} E(f(B_i \cup x) - f(B_i)) \right)
\]

\[
\geq \frac{1}{k} \sum_{j=1}^{l} \gamma_{B_i \cup S_j \cup B_i} E(f(B_i \cup S_j) - f(B_i))
\]

\[
\geq \frac{1}{k} \sum_{j=1}^{l} \gamma_{B_i \cup S_j \cup B_i} E(f(S_j) - f(B_i))
\]

\[
\geq \frac{\gamma_{B_i \cup S_j \cup B_i}}{k} \min E(f(S_j) - f(B_i)).
\]

For proving Lemma 3 we require another auxillary result.

Lemma 11. For any \( x \in A \), \( P(x \in \cup_{j \in [l]} G_j) = \frac{1}{4} \sum_{j} P(x \in S_j) \).

Proof. We have

\[
P(x \in \cup_{j \in [l]} G_j) \\
= \sum_{j} P(x \in A_j \cap x \in \text{GREEDY}(A_i, k)) \\
= \sum_{j} P(x \in A_j) P(x \in \text{GREEDY}(A_i, k) | x \in A_i) \\
= \sum_{j} P(x \in A_j) P(x \in S_i) \\
= \frac{1}{4} P(x \in S_i).
\]

We now prove Lemma 3

Lemma 3. \( \exists j \in [l], E[f(G)] \geq (1 - \frac{1}{e^{\log \frac{1}{s}}}) f(S_j) \).

Proof. For \( i \in [k] \), let \( B_i : \text{GREEDY}(\cup_{j \in [l]} G_j, i) \), so that \( B_k = G \) in step 3 of Algorithm 2. Then,

\[
E[f(B_{i+1}) - f(B_i)] \\
\geq \frac{1}{k} \sum_{x \in A^*} P(x \in \cup_{j \in [l]} G_j) E[f(x \cup B_i) - f(B_i)]
\]

\[
\geq \frac{1}{k} \sum_{j=1}^{l} \left( \sum_{x \in S_j} E(f(B_i \cup x) - f(B_i)) \right)
\]

\[
\geq \frac{1}{k} \sum_{j=1}^{l} \gamma_{B_i \cup S_j \cup B_i} E(f(B_i \cup S_j) - f(B_i))
\]

\[
\geq \frac{1}{k} \sum_{j=1}^{l} \gamma_{B_i \cup S_j \cup B_i} E(f(S_j) - f(B_i))
\]

\[
\geq \frac{\gamma_{B_i \cup S_j \cup B_i}}{k} \min E(f(S_j) - f(B_i)).
\]

Using \( \gamma_{B_i \cup S_j \cup B_i} \geq \gamma_{S_j} \), and proceeding now as in the proof of
Theorem 2 we get the desired result.

\[
\-box
\]

A.2 Stochastic Greedy

Lemma 4. Let \( A, B \subset [n], \) with \( |B| \leq k \). Consider another
set \( C \) drawn randomly from \([n] \setminus A\) with \( |C| = \left\lceil \frac{n \log 1/s}{k} \right\rceil \).
Then

\[
E[\max_{v \in C} f(v \cup A) - f(A)] \geq \left( 1 - \frac{\delta}{k} \right) f(B) - f(A)
\]

Proof. To relate the best possible marginal gain from \( C \) to
the total gain of including the set \( B \setminus A \) into \( A \), we must upper bound the probability of overlap between \( C \) and \( B \setminus A \) as follows:

\[
P(C \cap (B \setminus A) \neq \emptyset) = 1 - \left( 1 - \frac{|B \setminus A|}{|n| - |A|} \right)^{|C|}
\]

\[
= 1 - \left( 1 - \frac{|B \setminus A|}{|n| - |A|} \right)^{\left\lceil \frac{n \log 1/s}{k} \right\rceil}
\]

\[
\geq 1 - \exp \left( - \frac{n \log 1/s}{k} \frac{|B \setminus A|}{|n| - |A|} \right)
\]

\[
\geq 1 - \exp \left( - \frac{|B \setminus A| \log 1/s}{k} \right)
\]

\[
\geq (1 - \frac{\delta}{k}) \frac{|B \setminus A|}{k} \left( 1 - \frac{|B \setminus A|}{k} \right)
\]

where (14) is because \( \frac{|B \setminus A|}{k} \leq 1 \). Let \( S = C \cap (B \setminus A) \). Since
\[
f(v \cup A) - f(A) \text{ is nonnegative,}
\]
\[
E[\max_{v \in C} f(v \cup A) - f(A)]
\geq P(S \neq \emptyset)E[\max_{v \in C} f(v \cup A) - f(A)|S \neq \emptyset]
\geq (1 - \delta)\frac{|B \setminus A|}{k}E[\max_{v \in C \cap (B \setminus A)} f(v \cup A) - f(A)|S \neq \emptyset]
\geq (1 - \delta)\frac{|B \setminus A|}{k}\sum_{v \in B \setminus A} \frac{f(v \cup A) - f(A)}{|B \setminus A|}
\geq (1 - \delta)\frac{|A \cap B \setminus A|}{k}(f(B) - f(A)).
\]

\textbf{A.3 Linear regression}

\textbf{Lemma A.6} For the maximization of the R^2 (7) ν_S ≥ \lambda_{\text{max}(C_S)} \lambda_{\text{max}(C_S)}$, where C_S is the submatrix of C with rows and columns indexed by S.

\textit{Proof.} Say A, B is an arbitrary partition of S. Consider, 
\[
\|P_{AY}\|_2^2 = y^T P_A y
= y^T X_A (X^T_A X_A)^{-1} X^T_A y
\geq \|X^T_A y\|_2^2 \lambda_{\text{min}} ((X^T_A X_A)^{-1})
= \frac{\|X^T_A y\|_2^2}{\lambda_{\text{max}} (X^T_A X_A)}
\geq \|X^T_A y\|_2^2 \frac{1}{\lambda_{\text{max}} (X^T_S X_S)}.
\]

where (15) results from the fact that all orthogonal projection matrices are symmetric and idempotent. Repeating a similar analysis for B instead of A, we get 
\[
\|P_{AY}\|_2^2 + \|P_{BY}\|_2^2 \geq \frac{\|X^T_A y\|_2^2 + \|X^T_B y\|_2^2}{\lambda_{\text{max}} (X^T_S X_S)}
= \frac{\|X^T_A y\|_2^2}{\lambda_{\text{max}} (X^T_S X_S)}.
\]

A similar analysis also gives \(\|P_{S \setminus Y}\|_2^2 \leq \frac{\|X_S y\|_2^2}{\lambda_{\text{min}} (X_S X_S)}\), which gives the desired result. \hfill \Box

\textbf{A.4 RSC implies weak subadditivity}

Let \(\beta^{(S)} := \max_{\supp(x) \subseteq S} g(x)\).

\textbf{Lemma A.8} For a support set \(S \subset [d]\), \(f(S) \geq \frac{1}{2\pi} \|\nabla g(0)\|_S^2\).

\textit{Proof.} For any \(v\) with support in \(S\), 
\[
g(\beta^{(S)}) - g(0) \geq g(v) - g(0)
\geq \langle \nabla g(0), v \rangle - \frac{L}{2} \|v\|_2^2.
\]

Using \(v = \frac{1}{L} \nabla g(0)\), we get the desired result. \hfill \Box

\textbf{Lemma A.9} For any support set \(S\), \(f(S) \leq \frac{1}{2m} \|\nabla g(0)\|_S^2\).

\textit{Proof.} By strong concavity, 
\[
g(\beta^{(S)}) - g(0) \leq \langle \nabla g(0), \beta^{(S)} \rangle - \frac{m}{2} \|\beta^{(S)}\|_2^2
\leq \max_v \langle \nabla g(0), v \rangle - \frac{m}{2} \|v\|_2^2,
\]
where \(v\) is an arbitrary vector that has support only on \(S\). Optimizing the RHS over \(v\) gives the desired result. \hfill \Box

\textbf{B Additional experiments}

Figures 4 and 5 shows the performance of all algorithms on the following metrics: log likelihood (normalized with respect to a null model), generalization to new test measurements from the same true support parameter, area under ROC, and percentage of the true support recovered for \(l = 2\). Recall that Figure 1 presents the results from the same experiment with \(l = 10\). Clearly, the greedy algorithms benefit more from increased number of partitions.

![Figure 4: Distributed linear regression, \(l = 2\) partitions, \(n = 800\) training and test samples, \(\alpha = 0.5\). Training/testing performance](image)

![Figure 5: Generalization accuracy vs number of features selected](image)
Figure 5: Distributed linear regression, $l = 2$ partitions,
$n = 800$ training and test samples, $\alpha = 0.5$. Support
Recovery Performance