Submodularity in Statistics: Comparing the Success of Model Selection Methods

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Abstract

We demonstrate the usefulness of submodularity in statistics as a characterization of the difficulty of the search problem of feature selection. The search problem is the ability of a procedure to identify an informative set of features as opposed to the performance of the optimal set of features. Submodularity arises naturally in this setting due to its connection to combinatorial optimization. In statistics, submodularity isolates cases in which collinearity makes the choice of model features difficult from those in which this task is routine. Researchers often report the signal-to-noise ratio to measure the difficulty of simulated data examples. A measure of submodularity should also be provided as it characterizes an independent component difficulty. Furthermore, it is closely related to other statistical assumptions used in the development of the Lasso, Dantzig selector, and sure information screening.

1 Introduction

We study the problem of selecting predictive features from a large feature space. Our data consists of $n$ observations of (response, feature) sets, $(y_i, x_{i1}, \ldots, x_{im})$, where each
observation has \( m \) associated features. Observations are collected into matrices and the following model is assumed for our data

\[
Y = X\beta + \epsilon
\]  
\[
\epsilon \sim N_n(0, \sigma^2 I_n)
\]

(1)

where \( X \) is an \( n \times m \) matrix and \( Y \) is an \( n \times 1 \) response vector. Typically, most of the elements of \( \beta \) are 0. Hence, generating good predictions requires identifying the small subset of predictive features. The model (1) proliferates the statistics and machine learning literature. In modern applications, \( m \) is often large, potentially with \( m \gg n \), which makes the selection of an appropriate subset of these features essential for prediction.

The model selection problem is to minimize the error sum of squares

\[
\text{ESS}(\hat{Y}) = \|Y - \hat{Y}\|^2_2 = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2
\]

while restricting the number of nonzero coefficients:

\[
\min_{\beta} \text{ESS}(X\beta) \quad \text{s.t.} \quad \|\beta\|_0 = \sum_{i=1}^{m} I_{\{\beta_i \neq 0\}} \leq k,
\]

(2)

where the number of nonzero coefficients, \( k \), is the desired sparsity. Note that we are not assuming a sparse representation exists, merely asking for a sparse approximation.

In the statistics literature, the model selection problem (2) is more commonly posed as a penalized regression:

\[
\hat{\beta}_{0,\lambda} = \arg\min_{\beta} \{ \text{ESS}(X\beta) + \lambda \|\beta\|_0 \}
\]

(3)

where \( \lambda \geq 0 \) is a constant. The classical hard thresholding algorithms \( C_p \) (Mallows, 1973), AIC (Akaike, 1974), BIC (Schwarz, 1978), and RIC (Foster and George, 1994) vary \( \lambda \).

The solution to (3) is the least-squares estimator on an optimal subset of features. Let \( M \subset \{1, \ldots, m\} \) indicate the coordinates of a given model so that \( X_M \) is the corresponding submatrix of the data. If \( M^{\ast}_{\lambda} \) is the optimal set of features for a given \( \lambda \) then \( \hat{\beta}_{0,\lambda}^{\ast} = \)
\[(X_{M^*}^T X_{M^*})^{-1}X_{M^*}Y.\]

Given the combinatorial nature of the constraint, solving (2) quickly becomes infeasible as \(m\) increases and is NP-hard in general (Natarajan, 1995). Forward stepwise is the greedy approximation to the solution of (2). Let \(M_i\) be the features in the forward stepwise model after step \(i\) and note that the size of the model is \(|M_i| = i\). The algorithm is initialized with \(M_0 = \emptyset\) and iteratively adds the variable which yields the largest reduction in ESS. Hence, \(M_{i+1} = \{M_i \cup j\}\) where

\[ j = \arg \max_{l \in \{1,\ldots,m\} \setminus M_i} \text{ESS}(X_{M_i \cup l} \hat{\beta}_{M_i \cup l}^{LS}). \]

After the first feature is selected, subsequent models are built having fixed that feature in the model. \(M_1\) is the optimal size-1 model, but \(M_i\) for \(i \geq 2\) is not guaranteed to be optimal, because \(M_i\) is forced to include the features identified at previous steps.

Subset selection problems are difficult because features can interact in unexpected ways. Here, “unexpected” means that the change in model fit when adding a feature can be completely different depending on the other features in the model. This paper characterizes the cases in which features produce such unexpected results.

A simple example from Miller (2002) clarifies this point. Suppose forward stepwise is run on the data in Table 1. The first step selects the feature that is maximally correlated with \(Y\). For features \(X_1, X_2,\) and \(X_3,\) these are \(r_{Y1} = .0, r_{Y2} = -.0016,\) and \(r_{Y3} = .4472,\) respectively. Therefore, forward stepwise selects \(X_3\) on the first step. The second step chooses the feature with the maximum partial correlation. That is, the maximum correlation when features are considered orthogonally to \(X_3.\) For \(X_1\) and \(X_2\) these are \(r_{Y1,3} = .0\) and \(r_{Y2,3} = -.0014,\) respectively. Forward stepwise appears to find a significant feature on the first step, but then no other features seem important. The true equation for the response, however, is \(Y = X_1 - X_2.\) This cannot be identified by forward stepwise because of the “incorrect” first step which includes \(X_3.\) Furthermore, unless forward stepwise continues to select features even when they appear uninformative, the optimal set can never be found. Intuitively, the difficulty arises because \(X_1\) and \(X_2\) have large errors which cancel out.
Table 1: Simple data in which forward stepwise fails to identify the correct model.

| Y  | $X_1$ | $X_2$ | $X_3$ |
|----|-------|-------|-------|
| -2 | 1000  | 1002  | 0     |
| -1 | -1000 | -999  | -1    |
| 1  | -1000 | -1001 | 1     |
| 2  | 1000  | 998   | 0     |

Most of our discussion concerns maximizing the model fit as opposed to minimizing loss. Let $[m] = \{1, \ldots, m\}$. For a subset of indices $S \subset [m]$, we denote the corresponding columns of our data matrix as $X_S$, or merely $S$ when the overloaded notation will not cause confusion. Our measure of model fit for a set of features $X_S$ is the coefficient of determination, $R^2$, defined as

$$R^2(S) = 1 - \frac{\text{ESS}(X_S \hat{\beta}_S)}{\text{ESS}(\bar{Y})}$$

where $\bar{Y}$ is the constant vector of the mean response and $\hat{\beta}_S$ is the least squares estimate of $\beta_S$.

Forward stepwise performs well when the improvement in fit obtained by adding a set of features to a model is upper bounded by the sum of the improvements of adding the features individually. If a set of features improves the model fit when considered together, a subset of those features must improve the fit as well. Consider the improvement in fit by adding $X_S$ to the model $X_T$:

$$\Delta_T(S) := R^2(S \cup T) - R^2(T).$$

Letting $S = A \cup B$, bound $\Delta_T(S)$ as

$$\Delta_T(A) + \Delta_T(B) \geq \Delta_T(S). \quad (4)$$

If $A \cup B$ improves the model fit, equation (4) requires that either $A$ or $B$ improve the fit when considered in isolation. Therefore, signal that is present due to complex relationships among features cannot be completely hidden when considering subsets of...
these features. Equation (4) defines a submodular function:

**Definition 1 (Submodular Function).** Let $F : 2^{|m|} \rightarrow \mathbb{R}$ be a set function defined on the power set of $[m]$. $F$ is submodular if $\forall A, B \subset [m]$

$$F(A) + F(B) \geq F(A \cup B) + F(A \cap B) \quad (5)$$

The intuition in equation (4) is recovered by considering $A \cap B = \emptyset$. Alternatively, Definition 1 can be rewritten as

$$F(A) - F(A \cap B) + F(B) - F(A \cap B) \geq F(A \cup B) - F(A \cap B)$$

$$\Rightarrow \Delta_{A \cap B}(A) + \Delta_{A \cap B}(B) \geq \Delta_{A \cap B}(A \cup B),$$

which considers the impact of $A \setminus B$ and $B \setminus A$ given $A \cap B$. The influence of the union of set differences is less than the impact of the sum of their marginal influences. We will refer to data as being submodular if $R^2$ is a submodular function on the data.

Forward selection is a natural algorithm under submodularity as it adds the feature to the model that yields the maximum marginal increase in fit. To fix notation, if $S_i$ is the model at step $i$, feature $X_j$ is added if

$$j = \arg\max_{l \in S_i} \Delta_{S_i}(X_l)$$

and $S_{i+1} = \{S_i \cup j\}$. Other greedy procedures have been proposed that change the criteria being maximized at each step. For different criteria, this yields orthogonal matching or orthogonal projection pursuit (Barron et al., 2008; Miller, 2002).

For all such methods, let $\hat{Y}^{(k)} = X_{S_k} \hat{\beta}_{S_k}$ be the estimated response after $k$ steps of the algorithm. Previous analyses determined the rate at which $\text{ESS}(\hat{Y}^{(k)})$ decreases as a function of $k$ (Barron et al., 2008; Jaggi, 2013). Instead, we focus on identifying the data conditions that guarantee that $\text{ESS}(\hat{Y}^{(k)})$ is close to that of the optimal size $k$ subset. If forward stepwise is used and $R^2$ is submodular, the classic result of Nemhauser et al. (1978) shows that $R^2(S_k) \geq (1 - 1/e)R^2(S_k^*)$, where $S_k^*$ is the subset of features which
solves the sparse regression problem in equation (2).

Instead of asking for an approximate solution to (3), one can relax the problem formulation. For example, the $l_0$ penalty can be relaxed to an $l_1$ penalty, yielding the Lasso (Tibshirani, 1996). Additionally, loss be measuring with the $l_\infty$ norm, which yields the Dantzig selector (Candes and Tao, 2007). While subset selection and greedy methods like forward stepwise are classically studied, these relaxations have been the primary focus of research in recent years. For cases where $\log(p) = O(n^c)$ for $c > 0$, the computational improvements from relaxing the constraint in equation (2) do not produce efficient algorithms. In these cases, a feature screening method can be used to reduce the dimensionality $p$ to feasible ranges before performing model selection (Fan and Lv, 2008).

These define two classes of algorithms: the first maintains the problem formulation in (2) and provides approximate solutions, while the provides exact solutions to relaxed problem formulations. Given that both classes of algorithms can be used to answer the same question, it is natural to ask which style of approximation is preferred. A general framework comparing these as penalized regressions is given in Fan and Li (2001), and cases in which approximating (2) is preferable to solving the relaxations are discussed in Johnson et al. (2015a). We take a different approach and analyze the assumptions necessary to have performance guarantees for either class of methods.

Our main contribution is a characterization of the data situations which are difficult for feature selection algorithms. This characterization should provide statistical insight as well as a way to generalize insight gained from low-dimensional problems. Unfortunately these two are not accomplished in the same way, which necessitates providing multiple definitions of approximate submodularity.

Das and Kempe (2011) introduced a notion of approximate submodularity, measured by the submodularity ratio, which we will call “statistical submodularity” given its connection to performance guarantees of statistical algorithms. We provide a characterization of the data situations in which this criteria holds. While the submodularity ratio is statistically useful, it does not allow insight gained from low-dimensional problems...
to be generalized. We provide a stronger definition for approximate submodularity and show that it yields a lower bound on the submodularity ratio. In particular, we explain which data conditions yield approximate submodularity for all feasible two-dimensional regression problems. While this is restrictive, it yields generalizable bounds and insights.

As submodularity is a function of model fit, it depends on the response $Y$. This allows for a broader understanding of problematic correlation structures and is highly relevant to many simulation settings. From this perspective, not all deviations from orthogonality are the same. Spectral measures of such deviations do not always account for this lack of symmetry. Often simulations are described by their signal to noise ratio without considering the relative difficulty of different functional forms of the response. Provide an honest measurement of the difficulty of simulated data case requires considering both the strength of the signal and the ease with which the signal can be found.

Lastly, we demonstrate that submodularity often appears in statistics literature, just not by that name. We discuss the restricted eigenvalue (Raskutti et al., 2010) and conditions for sure independent screening (SIS) (Fan and Lv, 2008). The discussion highlights the data situations in which the sparse regression problem (2) is solvable by either approximating the solution or relaxing the problem formulation. Essentially, achieving an approximate solution to the exact problem is successful is the same instances in which achieving an exact solution to the approximate problem is successful. Furthermore, counter-intuitive results from recent conditional testing literature on forward stepwise and Lasso (Taylor et al., 2014) are explained by deviations from submodularity.

Section 2 introduces submodularity and our definition of approximate submodularity. Section 3 provides a simple example with only two features to provide intuition about the constraint of approximate submodularity. Furthermore, it is shown how submodularity can influence the search path identified by a greedy procedure. We also demonstrate the effect of signal strength in conjunction with submodularity. If the signal is strong enough, deviations from submodularity are easier to tolerate because signal is harder to hide in complex relationships between features. Lastly, Section 4 discusses the connection between submodularity and more common assumptions in statistics.
2 Submodularity

Submodularity is a condition under which greedy algorithms perform well. In this section, submodularity is given a statistical interpretation which begins to reveal its relevance in statistics. We often need to consider a feature \( X_i \) orthogonal to those currently in the model, \( X_S \). This is referred to as adjusting \( X_i \) for \( X_S \). The projection operator (hat matrix), \( H_{X_S} = H_S = X_S(X_S^T X_S)^{-1} X_S^T \), projects a vector onto the span of the columns of \( X_S \). Therefore, \( X_i \) adjusted for \( X_S \) is denoted as residual \( X_{i,S^\perp} = (I - H_{X_S})X_i \). This same notation holds for sets of features: \( X_A \) adjusted for \( X_S \) is \( X_{A,S^\perp} = (I - H_{X_S})X_A \).

While assuming \( R^2 \) is submodular is uncommon in the statistics literature, an equivalent formulation has been discussed in the social science literature: the absence of conditional suppressor variables (Das and Kempe, 2008). It is often observed features that have positive marginal correlation with the response can have negative partial correlation in the presence of other features. Similarly, features can be more significant in the presence of others than they are in isolation. In these situations, “suppression” is said to have occurred. The words “suppression” and “suppressor variable” can be understood through the algebra of adjustment for multiple regression coefficients.

If \( X \) and \( Y \) are standardized, the coefficient for a feature \( X_i \) in a simple regression is the correlation between \( X_i \) and \( Y \): \( r_{Y,i} \). Letting \( C = S \setminus i \) be the other features in the model, the coefficient for \( X_i \) in a multiple regression is

\[
\hat{\beta}_i = \frac{\langle Y, X_i, C^\perp \rangle}{\langle X_i, C^\perp, X_i, C^\perp \rangle}.
\]

Therefore suppression occurs when variability in the feature of interest that is unrelated to \( Y \) is suppressed by the other features in the model.

A suppressor variable is one which, once controlled for, increases the observed significance of another feature. The absence of a conditional suppressor implies that \( \forall S \subseteq [m] \) and \( i, j \notin S \)

\[
|\text{Corr}(Y, X_{i,(S\cup j)^\perp})| \leq |\text{Corr}(Y, X_{i,(S)^\perp})|.
\]
Suppression is fundamentally the same problem as Simpson’s paradox and Lord’s paradox. The distinction arises based on the type of features being considered. Given features $X_1$ and $X_2$, Simpson’s paradox can occur when both features are categorical, Lord’s paradox can occur when one is categorical and the other is numeric, and suppression can occur when both features are numeric. Any of these paradoxes create problems with interpreting the influence of features in a regression model.

If one is only interested in prediction, the interpretation of coefficients is often unimportant. The existence of a suppressor variable does not change the predictions from a model; however, suppression has significant consequences for the ability of an algorithm to identify an important feature. In extreme cases, important features can only be identified as such in the context of many other features. To extend the simple example given in the introduction, consider the following set of random variables:

$$Z = N_p(0, \sigma_z I_p)$$
$$\epsilon = N_{p-1}(0, \sigma_\epsilon I_{p-1})$$
$$X_{1:(p-1)} = Z_{1:(p-1)} + \epsilon$$
$$X_p = Z_p - \sum_{i=1}^{p-1} \epsilon_i$$
$$Y = \sum_{i=1}^{p} X_i = \sum_{i=1}^{p} Z_i$$

Suppose that $\sigma_\epsilon/\sigma_z$ is large enough that the variability in $\epsilon$ hides any signal that is in $Z_i$. In this example, any model with fewer than $p$ features has an $R^2$ near 0, while using all $p$ features yields an $R^2$ of 1. The improvement in fit by adding any single variable is approximately 0 or 1, depending on which other variables are in the model. This clearly harms any procedure that solves isolated subproblems. Given the equivalence between lack of suppression and submodularity, we will use these term interchangeably. Similarly, subsets of features which violate Definition 1 are instances of supermodularity. Therefore suppression situations are also supermodular.\(^1\) Further implications of the submodularity of $R^2$ are understood by considering equivalent definitions of submodular functions. Definition 1 provides the classical definition of submodularity, and two refinements can

\(^1\)Given that $R^2 \geq 0$, submodular function are also subadditive. Similarly, supermodular ones are superadditive. While we do not use this terminology, it may be encountered elsewhere.
be made that merely specify the sets under consideration in increasing detail. For completeness, all three formulations are provided in Definition 2 and are ordered in terms of specificity.

**Definition 2** (Submodularity). Let $F : 2^{[m]} \to \mathbb{R}$ be a set function defined on the the power set of $[m]$. $F$ is submodular iff

1. *(Definition)* $\forall A, B \subset [m]$\[ F(A) + F(B) \geq F(A \cup B) + F(A \cap B) \]
   $\Rightarrow F(A) - F(A \cap B) \geq F(A \cup B) - F(B)$
   $\Rightarrow \Delta_{A \cap B}(A) \geq \Delta_B(A)$

2. *(First-order difference)* $\forall A, B$ such that $A \subset B \subset [m]$ and $i \in [m] \setminus B$\[ F(A \cup \{i\}) - F(A) \geq F(B \cup \{i\}) - F(B) \]
   $\Rightarrow \Delta_A(i) \geq \Delta_B(i)$

3. *(Second-order difference)* $\forall A \subset [m]$ and $i, j \in [m] \setminus A$\[ F(A \cup \{i\}) - F(A) \geq F(A \cup \{i, j\}) - F(A \cup \{j\}) \]
   $\Rightarrow \Delta_A(i) \geq \Delta_{A \cup \{j\}}(i)$

The definition in terms of first-order differences shows that submodular functions are similar to concave functions in that they exhibit diminishing marginal returns. The marginal impact or discrete derivative of adding a feature to $A$ is larger than that of adding it to $B$ since $A \subset B$. In terms of optimization, however, they behave like convex functions and can be efficiently minimized. See Bach (2011) for a survey of this viewpoint. One further simplification is possible by specifying $B = A \cup \{j\}$, which yields the definition in terms of second-order differences. This provides the most granular, well-specified definition of submodularity, and it is the easiest to verify in practice. The proofs of the equivalence of these definitions are standard and can be found in many places, for example
Bach (2011). Furthermore, when showing the equivalence of definitions for approximate submodularity, we will be using proofs of essentially the same form.

In statistical terms, the first- and second-order difference definitions capture the intuitive notion that correlated features share information. Suppose $X_S$ is a highly positively correlated set of features where $\beta_i \geq 0, \forall i \in S$. If only $X_j, j \in S$, is added to the model, it produces a larger marginal improvement in fit than if the entire set $X_S$ is included: $\Delta_{\emptyset}(X_j) \geq \Delta_{S \setminus j}(X_j)$. This claim does not hold in general, but does in this example because it is submodular. Correlation structures which violate this intuitive notion of shared information are described in Section 3.1.

The above discussion follows from elementary decompositions of simple and multiple regression coefficients. Let $S = \{i \cup j\}$ and consider the following models, where subscripts $m$ and $s$ index the model coefficients and error terms:

|                       | Multiple Regression                      | Simple Regression                      |
|-----------------------|-----------------------------------------|----------------------------------------|
| Model                 | $Y = \beta_{0,m} + X_i \beta_{i,m} + X_j \beta_{j,m} + \epsilon_s$ | $Y = \beta_{0,s} + X_i \beta_{i,s} + \epsilon_m$ |
| Estimated Coefficients| $\hat{\beta}_{0,m}, \hat{\beta}_{i,m}$ and $\hat{\beta}_{j,m}$ | $\hat{\beta}_{0,s}$ and $\hat{\beta}_{i,s}$ |

The simple regression coefficient can be decomposed into direct and indirect effects:

$$\hat{\beta}_{i,s} = \hat{\beta}_{i,m} + \hat{\alpha}_j \hat{\beta}_{j,m}. \quad (6)$$

where $\hat{\alpha}_j$ is estimated from

$$X_i = \alpha_0 + X_j \alpha_j + \epsilon.$$

By construction, all terms are positive in equation (6) and the simple regression coefficient $\hat{\beta}_{i,s}$ is larger than $\hat{\beta}_{i,m}$. Therefore, the marginal impact of adding $X_i$ is larger in isolation than in conjunction with $X_j$. While this is a simplistic example, it introduces the general insight gained in later sections. In the simplest case, submodular data requires positively correlated features to have correlations with the response of the same sign. For example, both must be negative or positive. Similarly, if features are negatively correlated, their correlations with the response need to be of opposite sign.

The conditions provided in Definition 2 need to be relaxed in order to capture the
continuum of possible scenarios. This will provide a measure of how signal can “hide” in sets of features while not being visible marginally. This measure is closely connected to assumptions more commonly discussed in statistics (see Section 4). There are two conflicting interests when providing an approximate definition of submodularity. First, it needs to be statistically meaningful. Such a definition should characterize a relevant statistical problem that needs to be addressed by many algorithms. Second, understanding submodularity in spaces with few features should provide generalizable insight into higher-dimensional problems. Unfortunately, both goals are not accomplished in the same way. Therefore, two notions of approximate submodularity are developed and their relationships are described.

Forward stepwise works better if the influence of a set $S$ can be bounded by the sum of the margin influences of the elements in it. This can be achieved by applying Definition 1 multiple times to reduce the left hand side to a sum of individual elements. If $A = \{a_1, \ldots, a_l\} \subset [m]$ and $B = \{b_1, \ldots, b_m\} \subset [m]$, this yields

$$\sum_{i=1}^{l} \Delta_{A \cap B}(a_i) + \sum_{i=1}^{m} \Delta_{A \cap B}(b_i) \geq \Delta_{A \cap B}(A \cup B).$$

(7)

Note that for elements $a_i \in A \cap B$ or $b_j \in A \cap B$ that $\Delta_{A \cap B}(a_i) = \Delta_{A \cap B}(b_j) = 0$.

Das and Kempe (2011) propose a definition of approximate submodularity that requires equation (7) to hold approximately by including a constant $\gamma > 0$ on the right hand side. This is different than incorporating the same constant into Definition 1 as multiple applications of the definition are required to produce equation (7).

For additional simplicity, consider adding the set $A = \{a_1, \ldots, a_l\} \subset [m]$ to the model $S$. Hence $\Delta_S(a_i)$ is the marginal increase in $R^2$ by adding $a_i$ to model $S$. In this simple case, $\Delta_S(a_i)$ is the squared partial-correlation between the response $Y$ and $a_i$ given $S$: $\Delta_S(a_i) = \text{Cor}(Y, a_i \perp S)^2$. Therefore, define the vector of partial correlations as $r_{Y,A,S \perp} = \text{Cor}(Y, A,S \perp)$, then the left hand side of (7) is $\|r_{Y,A,S \perp}\|^2_2$. Similarly, if we define $C_{A,S \perp}$ as the correlation matrix of $A,S \perp$ then $\Delta_S(A) = r'_{Y,A,S \perp} C_{A,S \perp}^{-1} r_{Y,A,S \perp}$. 

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Definition 3. The submodularity ratio, \( \gamma_{sr} \), of \( R^2 \) with respect to a set \( S \) and \( k \geq 1 \) is

\[
\gamma_{sr}(S, k) = \min_{(T:T \cap S = \emptyset, |T| \leq k)} \frac{r'_{Y,T,S} r_{Y,T,S \perp}}{r'_{Y,T,S \perp} C_{T,S \perp}^{-1} r_{Y,T,S \perp}}
\]

The minimization identifies the worst case set \( T \) to add to the model \( S \). It captures how much \( R^2 \) can increase by adding \( T \) to \( S \) (denominator) compared to the combined benefits of adding its elements to \( S \) individually (numerator). \( R^2 \) is submodular if \( \gamma_{sr} \geq 1 \) for all \( S \subset [m] \) and \( k = 2 \). Only checking \( k = 2 \) is sufficient due to the second-order difference definition of submodularity and is clear from the proofs later in this section.

To not conflate the different notions of approximate submodularity introduced in this section, \( \gamma_{sr} \) will be referred to as the submodularity ratio or statistical submodularity. It can be used in proofs of the performance of greedy algorithms (Johnson et al., 2015b; Das and Kempe, 2011) and is lower bounded by a sparse eigenvalue (Das and Kempe, 2011). The connection to spectral quantities is obvious as \( \gamma_{sr} \) is an inverted Rayleigh quotient of the covariance matrix \( C_{T,L} \). As \( C_{T,L} \) is the Schur complement of \( C_{T \cup L} \), Corollary 2.4 from Zhang (2006) proves that \( \gamma_{sr} \) is lower bounded by the minimum eigenvalue of \( C_{T \cup L} \). The minimum sparse eigenvalue merely removes the dependence on the selected sets \( L \) and \( T \). The connections to other algorithms that depend on spectral quantities are discussed in Section 4.

The submodularity ratio is not appealing from the perspective of submodularity. It is redefined for different cardinalities \( k \) and does not allow information gained for fixed \( k \) to percolate to larger \( k \). We now provide a refined construction of approximate submodularity that produces generalizable insights. The definitions of approximate submodularity should mirror those of Definition 2, so that knowledge gained from restrictive, two-dimensional cases can generalize to higher-dimensional cases. These equivalent definitions, however, consider submodular functions in a slightly different context than the submodularity ratio \( \gamma_{sr} \). The distinction is due to bounding the minimum of a set of differences versus the sum of a set of differences. Clearly bounding the minimum is stronger.

Approximate submodularity is constructed by starting with the second-order differ-
ences definition as it is the most granular and well-specified. Ideally, the sum of the marginal impact of features considered individually would be approximately greater than their impact considered jointly. Namely, for some constant $\gamma > 0$,

$$
\Delta_A(i) + \Delta_A(j) \geq \gamma \Delta_A(i, j).
$$

(8)

This is $\gamma_{A,2}$ after fixing the sets being minimized, but is unfortunately too weak to generalize to the larger sets considered in Definition 2. Instead, we must maintain the type of comparisons considered in the standard definitions.

**Definition 4 (Approximate Submodularity).** $F$ is approximately submodular if there exists constants $\gamma_s, \gamma_{s2}$, where $\gamma_{s2} \geq \gamma_s > 0$, such that any of the following hold

1. **(Second order difference)** $\forall A \subset [m]$ and $i, j \in [m] \setminus A$

$$
F(A \cup \{i\}) - F(A) \geq \gamma_{s2}(F(A \cup \{i, j\}) - F(A \cup \{j\}))
$$

$$
\Rightarrow \Delta_A(i) \geq \gamma_{s2}\Delta_{A\cup j}(i)
$$

2. **(First order difference)** $\forall A, B$ such that $A \subset B \subset [m]$ and $i \in [m] \setminus B$

$$
F(A \cup \{i\}) - F(A) \geq \gamma_s(F(B \cup \{i\}) - F(B))
$$

$$
\Rightarrow \Delta_A(i) \geq \gamma_s\Delta_B(i)
$$

3. **(Definition)** $\forall A, B \subset [m]$

$$
F(A) - F(A \cap B) \geq \gamma_s(F(A \cup B) - F(B))
$$

$$
\Delta_{A \cap B}(A) \geq \gamma_s\Delta_B(A)
$$

One difference between the definitions for submodularity and approximate submodularity is that the constant will not be the same in all three cases, as indicated by our use of $\gamma_s$ and $\gamma_{s2}$; however, if either is strictly greater than 0, then they both are. We are most
interested in $\gamma_s$, which considers large sets, instead of $\gamma_{s2}$, which only holds for second order differences. We are able to provide a full account for $\gamma_{s2}$ though, which yields a conservative lower bound on $\gamma_s$. Therefore, understanding approximate submodularity in two dimensions gives generalizable insights. The equivalence of these definitions is proved in the Appendix.

It is easy to see that $\gamma_{sr} \geq \gamma_{s2}$ in the relevant region in which $\gamma_{s2} \leq 1$. In this region, forward stepwise can perform poorly. The second-order characterization of $\gamma_{sr}$ in equation (8) can be constructed using $\gamma_{s2}$.

$$\Delta_A(i) \geq \gamma_{s2} \Delta_{A \cup j}(i)$$

$$F(A \cup i) - F(A) \geq \gamma_{s2}(F(A \cup \{i, j\}) - F(A \cup \{j\}))$$

$$F(A \cup i) - F(A) + \gamma_{s2}(F(A \cup \{j\}) - F(A)) \geq \gamma_{s2}(F(A \cup \{i, j\}) - F(A))$$

$$\Rightarrow \Delta_A(i) + \Delta_A(j) \geq \gamma_s \Delta_A(i, j).$$

Where the last line follows since $\gamma_{s2} \leq 1$. The submodularity ratio fixes the base set; hence the above rearranges the definition of $\gamma_{s2}$ such that the marginal impact of all features is relative to the same base set $A$. This yields a bound on the sum of marginal effects, whereas the $\gamma_{s2}$ is a bound on the minimum of the marginal effects. As expected, the minimum can yield much worse bounds than the sum; however, as seen in Section (3.1), not all steps can be taken at this worst case bound.

### 3 Submodularity in 2 Dimensions

Attempting to classify types of suppression led Tzelgov and Henik (1991) to graph suppression situations that are possible with only two features. These graphs have unintuitive dimension, double-count data instances, and show impossible configurations. We analyze the same case, but provide graphs that fully characterize the set of possible regression problems. This clearly displays the regions in which $\gamma_{s2}$ and $\gamma_{sr}$ are bounded.
Figure 1: Characterization of possible two-dimensional regression problems: our data consists of $Y$, $X_1$, and $X_2$. $\hat{Y}_i$ is $Y$ projected on $X_i$. The side length from the origin to $\hat{Y}_i$ is $r_{Yi}$.

### 3.1 Graphing Approximate Submodularity

We parameterize possible regression problems using angles derived from projecting the response onto individual features. Our data consists of $Y$, $X_1$, and $X_2$ and $\hat{Y}_i$ as the response $Y$ projected onto $X_i$. See Figure 1 for an illustration. Since all features have been normalized, the distance from the origin to $\hat{Y}_i$ is the correlation between $Y$ and $X_i$, $r_{Yi}$. The correlation between explanatory features is parameterized as $\cos(\theta)$, where $\theta$ is the angle between $X_1$ and $X_2$. The relative predictive power of the features is measured by $\tau$, the angle between $\hat{Y}_1$ and $\hat{Y}_2$. Lastly, the strength of the signal is a function of the length of $b$, the side between $\hat{Y}_1$ and $\hat{Y}_2$.

Figures 2, 3, and 4 only display $\theta \in [0, \pi]$ and $r_{Yi} \geq 0$ because of the symmetries in submodularity. $\theta > \pi$ is equivalent to $\theta' = (2 - \theta)\pi \in [0, \pi]$ and $r_{Yi} = -r_{Yi}$ for some $i$.

The vertical axis has units $(\tau + \theta/2)\pi$ so that the contour plots are symmetric around $.5\pi$. Figure 1 is an isosceles triangle when $\tau + \theta/2 = .5\pi$, meaning that both features have the same marginal significance. Therefore, deviations correspond to one feature being marginally more significant than the other. Similarly, $\theta = .5\pi$ is the orthogonal case and represents one line of symmetry on the horizontal axis.

To completely specify the derived triangle in Figure 1, fix a measure of the signal to noise ratio as this does not represent a meaningful distinction between models for submodularity. Higher signal just means that the effects will be larger. This has the practical impact of being making it easier to identify a significant effect, but this discussion is de-
layed until Section 3.2. For convenience, we fix $R^2$ under the full model: $R^2_{full} = .5$. All figures are identical for any value of $R^2_{full} \in (0, 1]$. The length of $b$, the side between $\hat{Y}_1$ and $\hat{Y}_2$, is $\sqrt{(1 - r^2_{12})R^2_{full}}$.

Figure 2 is a contour plot of $\gamma_{s2}$ over the set of feasible regression problems. It demonstrates that submodularity ($\gamma_{s2} \geq 1$) is only possible when $\text{sign}(r_{12}r_{Y1}r_{Y2}) = 1$. This is the intuitive case introduced in Section 2: if features have opposing relationships with the response, we expect them to be negatively correlated. Since Figure 2 displays $r_{Y1} > 0$ and $r_{Y2} > 0$, submodularity only occurs when the features are positively correlated. Furthermore, for fixed $r_{12}$ the maximum $\gamma_{s2}$ occurs when both features have equal marginal effect. As this is a only a two-feature problem, the joint effects are also equal. Therefore, the common simulation setting that sets all non-zero coefficients to the same value maximizes the worse-case step, improving the performance of feature selection algorithms.

Figure 2 demonstrates that while submodularity holds in a large area, relaxing the definition does not increase the set of problems in a dramatic way; however, this is because $\gamma_{s2}$ is the single worst case step. Let $\gamma_i = \Delta(X_i)/\Delta_{X\backslash i}(X_i)$, $i \neq j$, $i, j \in \{1, 2\}$, then $\gamma_{s2}$ is calculated by

$$
\gamma_1 = \frac{r_{Y1}^2}{(r_{Y1}^2 - 2r_{Y1}r_{Y2}r_{Y2} + r_{Y2}^2r_{12}^2)/(1 - r_{12}^2)}
$$

$$
\gamma_2 = \frac{r_{Y2}^2}{(r_{Y2}^2 - 2r_{Y1}r_{Y2}r_{12} + r_{Y1}^2r_{12}^2)/(1 - r_{12}^2)}
$$

$$
\gamma_{s2} = \min(\gamma_1, \gamma_2).
$$

$\gamma_i$ is not symmetric in $X_1$ and $X_2$, though given our interest is in the true model containing both features, it is only important that one feature appears marginally significant. Importantly, both features cannot attain the minimum level $\gamma_{s2}$ simultaneously.

To illustrate this, consider bounding the marginal impact of both $X_1$ and $X_2$ using $\gamma_{s2}$. Summing these two inequalities produces

$$
\frac{\Delta_A(i) + \Delta_A(j)}{\Delta_{A\backslash ij}(i) + \Delta_{A\backslash ij}(j)} \geq \gamma_{s2}
$$

$$
\Rightarrow \frac{\Delta_A(i) + \Delta_A(j)}{2\Delta_A(i, j) - \Delta_A(i) - \Delta_A(j)} \geq \gamma_{s2},
$$

(9)
where the second line just rewrites the first such that the base set is constant. Figure 3 is a contour plot of the left hand side of equation (9). Clearly $\gamma_{s2}$ is a poor bound on this function, demonstrating that if signal is contained in the joint distribution of the features, it cannot be hidden from both marginal distributions simultaneously. It demonstrates that useful properties of submodularity obtain in much larger region than indicated by $\gamma_{s2}$ due to its conservativeness.

![Submodular Situations](image)

Figure 2: Contour plot of approximate submodularity using second order differences ($\gamma_{s2}$). Level sets are given for $\gamma_{s2} \in \{2, 4, \ldots, 1\}$.

Lastly, Figure 4 is a contour plot of the submodularity ratio $\gamma_{sr}$. It behaves similarly to the bound on the sum in Figure 3, though more regularly. There are several interesting features that can be seen from this graph. First, $\gamma_{sr}$ can be larger than 1. These are data situations in which forward stepwise achieves a better bound than the usual $(1 - 1/e)$ factor off of the optimal. This region corresponds to cases when the features are highly correlated and have similar marginal relationships with $Y$. In this case, there is redundancy in our data and selecting appropriate features is less difficult.

Second, the dependence of $\gamma_{sr}$ on $Y$ is captured by the vertical axis via $\tau$. Only orthogonal data, $\theta = .5\pi$, is submodular regardless of $Y$. In this case, the definition of
Figure 3: Contour plot of the left hand side of equation (3). The level sets are \( \{.2, .4, \ldots, 1\} \).

Submodularity, equation (5), holds with equality. This defines a modular function, and it is well known that the greedy algorithm produces the optimal answer when maximizing a modular function (Fujishige, 2005). Due to this dependence on \( Y \), \( \gamma_{sr} \) is not symmetric around the orthogonal case. Obviously the feasible region is not symmetric, but we consider symmetry in terms of the contours of \( \gamma_{sr} \). The minimum \( \gamma_{sr} \) along any vertical strip is achieved at the boundary of the feasible region. Along the boundaries, submodularity decays at the same rate when orthogonality is violated with by either positive or negative correlation. In this way, submodularity is symmetric around the orthogonal case. This demonstrates the result of Das and Kempe (2011), that \( \gamma_{sr} \) is lower bounded by minimum eigenvalues, which occur on the boundary of the feasible region.

3.2 Graphing Change in t-Statistics

We now address the issue of significant suppression. As the deviation from submodularity grows, the greedy search path can deviate from the optimal path; however, slight
Figure 4: This is a contour plot of the submodularity ratio over the set of feasible regression problems. Level sets are given for $\gamma_{sr} \in \{2, .4, \ldots , 2\}$.

suppression does not mean that the true model will not be found. For example, even
suppressed features may still be marginally significant enough to be identified. In this
case, the greedy search procedure has not been harmed.

To analyze these cases, the submodularity ratio can be related to differences in t-
statistics. As in Figure 4, consider the contours of the percentage change in t-statistics
caused by different correlation structures. For clarity, consider the following statistics:

$$
\beta_{1m} = r_{y1} \\
\beta_{1j} = \frac{r_{y1} - r_{y2r_{12}}}{1 - r_{12}^2} \\
t_{1m} = \frac{r_{y1}}{\sigma_{im}} \\
\sigma_{1m}^2 = \frac{1 - r_{y1}^2}{\sqrt{n - 1}} \\
t_{1j} = \frac{(r_{y1} - r_{y2r_{12}})}{(1 - r_{12}^2)^{1/2}\sigma_j} \\
\sigma_j^2 = \frac{1}{\sqrt{n - 1}} - \frac{r_{y1}^2 - 2r_{y1r_{y2r_{12}}} + r_{y2}^2}{\sqrt{n - 1(1 - r_{12}^2)}}
$$
Submodularity requires \( t_{1m}^2 \geq t_{1j}^2 \). This is a conservative statement since \( \frac{\sigma_{jm}^2}{\sigma_j^2} > 1 \).

If the features are jointly highly significant, this becomes very conservative because the ratio is much larger than 1.

\[
t_{m1}^2 = \frac{r_{y1}^2}{\sigma_m^2} \geq \frac{r_{y1}^2 - 2r_{y1}r_{y2}r_{12} + (r_{y2}r_{12})^2}{(1 - r_{12})\sigma_j^2} = t_{j1}^2
\]

\[
\Rightarrow r_{y1}^2 \geq \frac{r_{y1}^2 - 2r_{y1}r_{y2}r_{12} + (r_{y2}r_{12})^2}{1 - r_{12}^2}
\]

\[
\Rightarrow r_{y1}^2 + r_{y2}^2 \geq \frac{r_{y1}^2 - 2r_{y1}r_{y2}r_{12} + r_{y2}^2}{1 - r_{12}^2}
\]

Some algebra and incorporating \( \gamma_{sr} \) yields the following bound on the difference between the squared t-statistics:

\[
\Rightarrow t_{j1}^2 - t_{m1}^2 \leq \frac{(1 - \gamma_{sr})(r_{y1}^2 - 2r_{12}r_{y1}r_{y2} + r_{y2}^2)}{1 - r_{12}^2}
\]

The previous display ignores the symmetry of the problem: it is not of concern which of \( X_1 \) or \( X_2 \) is the suppressed feature, merely that there exists one. As such, add the corresponding equation for \( X_2 \) and divide by the sum of the marginal t-statistics. This treats \( X_1 \) and \( X_2 \) symmetrically, and yields

\[
\frac{t_{j1}^2 + t_{j2}^2}{t_{m1}^2 + t_{m2}^2} \leq 1 + \frac{2(1 - \gamma_{sr})(r_{y1}^2 - 2r_{12}r_{y1}r_{y2} + r_{y2}^2)}{(1 - r_{12}^2)(r_{y1}^2 + r_{y2}^2)}
\]

\[= 2\gamma_{sr}^{-1} - 1. \tag{10}\]

Since equation (10) is conveniently written in terms of the \( \gamma_{sr} \), we provide its contour plot in Figure 5. Equation (10) is always positive since \( \gamma_{sr} \leq 2 \).

The contours of Figure 5 are similar to those in Figure 4, but the contours change at different rates. If \( \gamma_{sr} > .8 \), then the ratio of squared t-statistics cannot be greater than 1.5. In this case, if a greedy procedure stops because all remaining features have a marginal t-statistic less than 2 in absolute value, neither feature can have a t-statistic larger than 3.46 when considered jointly. This upper bound is attained when one feature has a joint t-statistic of 0. If the joint information is split evenly between the two features,
the maximum joint t-statistics are 2.44. Again, it is important to note that $R^2$ is not involved in this equation. Therefore submodularity is measuring a fundamentally different component than the signal-to-noise ratio.

4 Connection to Other Assumptions

Some algorithms that leverage assumptions similar to submodularity are the Lasso, Dantzig selector, and sure independent screening (SIS). It should not be surprising that the Lasso and forward stepwise are closely connected as the LARS procedure demonstrates the approximate greedy nature of the Lasso (Efron et al., 2004). This similarity extends to the Dantzig selector given that the same assumption guarantees success of the Lasso and Dantzig selector (Bickel et al., 2009). Lastly, SIS needs guarantees that information learned from marginal correlations is sufficient for model selection (Fan and Lv, 2008). This section describes these procedures, the assumptions used to demonstrate their success, and their close connection to submodularity.
4.1 Lasso and Dantzig

Relaxing the constraint from problem (3) from $\|\beta\|_{l_0}$ to $\|\beta\|_{l_1}$ yields the Lasso problem (Tibshirani, 1996).

$$\hat{\beta}_l = \text{argmin}_{\beta} \{ \text{ESS}(X\beta) + \lambda \|\beta\|_{l_1} \}$$  \hspace{1cm} (11)

This is a convex program and can be efficiently solved using a variety of algorithms (Efron et al., 2004; Hastie and Junyang, 2014).

The Dantzig selector (Candes and Tao, 2007) optimizes the following linear program

$$\hat{\beta}_d = \text{argmin}_{\beta} \{ \|Y - X\beta\|_{\infty} + \lambda \|\beta\|_{l_1} \}$$  \hspace{1cm} (12)

Our discussion of these procedures focuses on the assumptions required to provide bounds on their prediction loss. Many properties have been defined such as the restricted isometry property (Candes and Tao, 2005), the restricted eigenvalue constant (Bickel et al., 2009; Raskutti et al., 2010), or the compatibility condition (van de Geer, 2007). For a review of these and related assumptions, see van de Geer and Buhlmann (2009). For our purposes, the most important of these is the restricted eigenvalue, which is defined over a restricted set of vectors that contain $\hat{\beta}_l$ and $\hat{\beta}_d$. Consider a subset $S \subset \{1, \ldots, p\}$ and constant $\alpha > 1$. Define the set

$$C(S; \alpha) := \{ \beta \in \mathbb{R}^p | \|\beta_S^c\|_1 \leq \alpha \|\beta_S\|_1 \}$$

The restricted eigenvalue of the $p \times p$ sample covariance matrix $\hat{\Sigma} = X^TX/n$ is defined over $S$ with parameter $\alpha \geq 1$.

$$\gamma_{re}^2(\alpha, S) := \min \left\{ \frac{\beta^T\hat{\Sigma}\beta}{\|\beta_S\|_2^2} : \beta \in C(S; \alpha) \right\}$$

If $\gamma_{re}$ is uniformly lower-bounded for all subsets $S$ with cardinality $k$, $\hat{\Sigma}$ satisfies a restricted eigenvalue condition of order $k$ with parameter $\alpha$. 
The restricted eigenvalue is effectively the submodularity ratio tailored to the Lasso and Dantzig selectors and generalized to hold for all response vectors \( Y \). Previous work has demonstrated the connection between \( \gamma_{sr} \) and sparse eigenvalues (Das and Kempe, 2011). A sparse eigenvalue with parameter \( k < p \) is

\[
\lambda_{\text{min}}(k) = \min_{\delta \in \mathbb{R}^k : 1 \leq \|\delta\|_0 \leq k} \frac{\delta^T X^T X \delta}{n \|\delta\|_2^2}.
\]

In order to remove the dependence on \( Y \) in the definition of \( \gamma_{sr} \), both the model \( S \) of size \( k \) and the comparison set \( L \) of size \( k \) need to be arbitrary. Therefore, \( \gamma_{sr}(S, k) \geq \lambda_{\text{min}}(2k) \). As discussed in Bickel et al. (2009), bounding the restricted eigenvalue bounds the minimum \( 2k \)-sparse eigenvalue. Thus the data conditions under which the Lasso and Dantzig selector are guaranteed to be successful are stronger than those under which forward stepwise is. Granted, the form of the guarantees are significantly different, but of interest is the similarity of the assumptions required.

The Lasso and Dantzig selector are known to over-estimate the support of \( \beta \) (Zou, 2006), and thus should not be compared to a sparse vector with \( k \) non-zero entries. The estimates \( \beta_l \) and \( \beta_d \) are elements of \( C(S; \alpha) \) with probability close to 1 (Bickel et al., 2009). Therefore, the bound corresponding to submodularity needs to minimize over \( C(S; \alpha) \) instead of truly sparse vectors. Given the looseness of \( \lambda_{\text{min}}(2K) \) as a lower bound on \( \gamma_{sr}(S, k) \), we expect a similar looseness exists between the restricted eigenvalue and the corresponding \( Y \)-dependent bound. While it is useful to provide guarantees that do not depend on \( Y \), the potential to produce a better estimate of the crucial constant at runtime may provide stronger practical performance guarantees. This development could mirror (Bertsimas et al., 2015).

### 4.2 SIS: Sure Independent Screening

SIS is a correlation learning method in which the marginal correlations between the response and all features are computed and the features with the largest \( d \) correlations are kept. This can be coupled with subsequent feature selection algorithms such as SCAD,
Dantzig, or Lasso to select a final model from these $d$ features. As an additional step, this process can be iterated in much the same way as stepwise regression: all remaining features are projected off of the selected set, and the process continues using the residuals from the first model. Therefore, iterated SIS is similar to a batch greedy method.

Fan and Lv (2008) split the assumptions for the asymptotic analysis into two groups: one focuses on parameters of the true regression function and the second focuses on the sampling distribution of the data. The assumptions on the true function are stronger than submodularity and the sampling distribution does not distort this. The most relevant assumption the authors make is the following:

**Assumption 1.** Fan and Lv (2008) For some $\kappa$, $0 \leq \kappa < 1/2$, and $c_2$, $c_3 > 0$,

$$\min_{i \in M_*} |\beta_i| \geq \frac{c_2}{n^{\kappa}} \quad \text{and} \quad \min_{i \in M_*} |\text{Cov}(\beta_i^{-1}Y, X_i)| \geq c_3.$$ 

This is of the same form as submodularity by:

$$|\text{cov}(\beta_i^{-1}Y, X_i)| = |\beta_i^{-1}| |\text{cov}(Y, X_i)| = |\beta_i^{-1}| |r_{Y_i}|,$$

where the second line follows because $X_i$ and $Y$ are standardized. As $r_{Y_i}$ is the coefficient estimate when $X_i$ considered marginally, Assumption 1 assures that features with non-zero coefficients in the true model have marginal correlations which are large enough to fall above the noise level. If $S$ is the true model, this can be written in a similar form as submodularity as $\Delta(X_i) \geq c_3 \Delta_{S\setminus i}(X_i)$. This is the first order difference definition of submodularity when $A = \emptyset$. Furthermore, this is more restrictive than statistical submodularity since $\gamma_{sr} > 0$ merely requires that there exists at least one feature which increases the model fit when considered in isolation. Assumption 1 requires that all true features increase model fit when considered in isolation. Therefore, all relevant joint information is visible from correlations. It is impossible to hide signal in even two-dimensional subproblems such as those considered in Section 3.
5 Conclusion

Submodularity plays an important role in statistics because it characterizes the difficulty of the search problem of feature selection. Assumptions used to prove the success of the Lasso, such as the restricted eigenvalue and restricted isometry properties, bound minimum sparse eigenvalues and hence are stronger assumptions than submodularity. Similarly, SIS requires true model features to have a bounded discrepancy between their joint coefficient in the true model and their marginal coefficient from a simple regression. Bounding this discrepancy is stronger than approximate submodularity as all true features cannot become vastly more significant in the presence of others. Similarly, worst case data examples can be crafted by intentionally breaking submodularity. This can be seen in Berk et al. (2013) and Miller (2002). Due to the importance of submodularity in discrete optimization, it provides a more theoretically robust assumption than those more commonly considered in statistics. Furthermore, it characterizes a different dimension of difficulty than the signal to noise ratio. As such, it is an important statistic to report in simulated data analyses.

6 Appendix

Proof of equivalence of Definition 2. Implications 3. \(\Rightarrow\) 2. \(\Rightarrow\) 1. are clear by appropriately defining the sets of interest as done when introducing the definitions of submodularity. To prove the reverse implications, we write lower-level definitions multiple times using nested sets. Summing these inequalities and simplifying gives the result.

To prove the first-order definition from the second-order definition, consider \(B = A \cup \{b_1, \ldots, b_k\}\), and apply the second-order definition to sets \(A'_i = A \cup \{b_1, \ldots, b_i\}\). This yields a set of inequalities

\[
\Delta_A(i) \geq \gamma s_2 \Delta_{A'_i}(i) \\
\Delta_{A'_i}(i) \geq \gamma s_2 \Delta_{A'_2}(i) \\
\vdots
\]

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\[ \Delta_{A_{k-1}}(i) \geq \gamma s_2 \Delta_B(i) \]
\[ \Rightarrow \Delta_A(i) \geq \gamma s_2 \Delta_B(i) + (\gamma s_2 - 1) \Delta_{A_1}(i) + \ldots + (\gamma s_2 - 1) \Delta_{A_{k-1}}(i) \]
\[ \geq \gamma s_2 \Delta_B(i) + \frac{\gamma s_2 - 1}{\gamma s_2} \Delta_A(i) + \ldots + \frac{\gamma s_2 - 1}{\gamma s_2}^{k-1} \Delta_A(i) \]
\[ \geq \left( \gamma s_2 + (1 - \gamma s_2) \frac{1 - \gamma s_2^{-k}}{1 - \gamma s_2} \right)^{-1} \Delta_B(i) \]

(13)

where the second to last line follows from applying the second order definition repeatedly to convert \( \Delta_{A_1'} \) to \( \Delta_A \). The constant in the last line provides a lower bound on \( \gamma s \) and is always strictly positive if \( \gamma s_2 \) is. It assumes that all of the individual steps are worst-case steps. As seen in Section 3.1, there are constraints on the number of steps that can be taken at this worst case level.

Similarly, to prove the standard definition from the first-order definition, apply the latter multiple times and sum the inequalities to produce \( \Delta_A(C) \geq \gamma s \Delta_B(C) \). Here \( C = \{c_1, \ldots, c_k\} \) and \( C \cap A = \emptyset \). Again, let \( A_1' = A \cup \{c_1, \ldots, c_i\} \). Note that since \( A \subset B \) this implies that \( B_1' = B \cup \{c_1, \ldots, c_i\} \). This yields a set of inequalities

\[ \Delta_A(c_1) \geq \gamma s \Delta_B(c_1) \]
\[ \Delta_{A_1'}(c_2) \geq \gamma s \Delta_{B_1'}(c_2) \]
\[ \vdots \]
\[ \Delta_{A_{k-1}}(c_k) \geq \gamma s \Delta_{B_{k-1}}(c_k) \]
\[ \Rightarrow \Delta_A(C) \geq \gamma s \Delta_B(C) \]

Where the last line follows by summing the previous lines, canceling most terms. \( \forall S, T \subset [m], \) set \( A = S \cap T, \) \( C = S \backslash T, \) and \( B = T. \) This yields the result.

\[ \square \]

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