Deep Submodular Functions

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Abstract

We start with an overview of a class of submodular functions called SCMMs (sums of concave composed with non-negative modular functions plus a final arbitrary modular). We then define a new class of submodular functions we call \textit{deep submodular functions} or DSFs. We show that DSFs are a flexible parametric family of submodular functions that share many of the properties and advantages of deep neural networks (DNNs), including many-layered hierarchical topologies, representation learning, distributed representations, opportunities and strategies for training, and suitability to GPU-based matrix/vector computing. DSFs can be motivated by considering a hierarchy of descriptive concepts over ground elements and where one wishes to allow submodular interaction throughout this hierarchy. In machine learning and data science applications, where there is often either a natural or an automatically learnt hierarchy of concepts over data, DSFs therefore naturally apply. Results in this paper show that DSFs constitute a strictly larger class of submodular functions than SCMMs, thus justifying their mathematical and practical utility. Moreover, we show that, for any integer $k > 0$, there are $k$-layer DSFs that cannot be represented by a $k'$-layer DSF for any $k' < k$. This implies that, like DNNs, there is a utility to depth, but unlike DNNs (which can be universally approximated by shallow networks), the family of DSFs strictly increase with depth. Despite this property, however, we show that DSFs, even with arbitrarily large $k$, do not comprise all submodular functions. We show this using a technique that "backpropagates" certain requirements if it was the case that DSFs comprised all submodular functions. In offering the above results, we also define the notion of an antitone superdifferential of a concave function and show how this relates to submodular functions (in general), DSFs (in particular), negative second-order partial derivatives, continuous submodularity, and concave extensions. To further motivate our analysis, we provide various special case results from matroid theory, comparing DSFs with forms of matroid rank, in particular the laminar matroid. Lastly, we discuss strategies to learn DSFs, and define the classes of deep supermodular functions, deep difference of submodular functions, and deep multivariate submodular functions, and discuss where these can be useful in applications.

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1 Introduction

Submodular functions are attractive models of many physical processes primarily because they possess an inherent naturalness to a wide variety of problems (e.g., they are good models of diversity, information, and cooperative costs) while at the same time they enjoy properties sufficient for efficient optimization. For example, submodular functions can be minimized without constraints in polynomial time [46] even though they lie within a $2^n$-dimensional cone in $\mathbb{R}^n$ and are parameterized, in their most general form, with a corresponding $2^n$ independent degrees of freedom. Moreover, while submodular function maximization is NP-hard, submodular maximization is one of the easiest of the NP-hard problems since constant factor approximation algorithms are often available — e.g., in the cardinality constrained case, the classic $1 - 1/e$ result of Nemhauser [113] via the greedy algorithm. Other problems also have guarantees, such as submodular maximization subject to knapsack or multiple matroid constraints [22, 21, 88, 66, 68].

Submodular functions are becoming increasingly important in the field of machine learning. In recent years, submodular functions have been used for representing diversity functions for the purpose of data summarization [91], for use as structured convex norms [6], for energy functions in tree-width unconstrained probabilistic models [48, 82, 67, 55], useful in computer vision [79], feature [98] and dictionary selection [33], viral marketing [58] and influence modeling in social networks [77], information cascades [89] and diffusion modeling [130], clustering [111], and active and semi-supervised learning [57], to name just a few. There also have been significant contributions from the machine learning community purely on the mathematical and algorithmic aspects of submodularity. This includes algorithms for optimizing non-submodular functions via the use of submodularity [110, 81, 71, 64], strategies for optimizing submodular functions subject to both combinatorial [65] and submodular level-set constraints [66], and so on.
One of the critical problems associated with utilizing submodular functions in machine learning and data science contexts is selecting which submodular function to use, and given that submodular functions lie in such a vast space with $2^n$ degrees of freedom, it is a non-trivial task to find one that works well, if not optimally. One approach is to attempt to learn the submodular function based on either queries of some form or based on data. This has led to results, mostly in the theory community, showing how learning submodularity can be harder or easier depending on how we judge what is being learnt. For example, it was shown that learning submodularity in the PMAC setting is fairly hard [10] although in some cases things are a bit easier [42]. Learning can be made easier if we restrict ourselves to learn within only a subfamily of submodular functions. For example, in [140, 92], it is shown empirically that one can effectively learn mixtures of submodular functions using a max-margin learning framework — here the components of the mixture are fixed and it is only the mixture parameters that are learnt, leading often to a convex optimization problem. In some cases, computing gradients of the convex problem can be done using submodular maximization [92], while in other cases, even a gradient requires minimizing a difference of two submodular functions [150].

Learning over restricted families rather than over the entire cone is desirable for the same reasons that any form of regularization in machine learning is useful. By restricting the family over which learning occurs, it decreases the complexity of the learning problem, thereby increasing the chance that one finds a good model within that family. This can be seen as a classic bias-variance tradeoff, where increasing bias can reduce variance. Up to now, learning over restricted families has apparently (to the authors' knowledge) been limited to learning mixtures over fixed components. This can be limited if the components are restricted, and if not might require a very large number of components. Therefore, there is a need for a richer and more flexible parametric family of submodular functions over which learning is not only still possible but ideally relatively easy. See Section 7.1 for further discussion on learning submodular functions.

In this paper, we introduce a new family of submodular functions that we term “deep submodular functions,” or DSFs. DSFs strictly generalize, as we show below, many of the kinds of submodular functions that are useful in machine learning contexts. These include the so-called “decomposable” submodular functions, namely those that can be represented as a sum of concave composed with modular functions [141].

We describe the family of DSFs and place them in the context of the general submodular family. In particular, we show that DSFs strictly generalize standard decomposable functions, thus theoretically motivating the use of deeper networks as a family over which to learn. Moreover, DSFs can represent a variety of complex submodular functions such as laminar matroid rank functions. These matroid rank functions include the truncated matroid rank function [52] that is often used to show theoretical worst-case performance for many constrained submodular minimization problems. We also show, somewhat surprisingly, that like decomposable functions, DSFs are unable to represent all possible cycle matroid rank functions. This is interesting in and of itself since there are laminar matroids that can not be represented by cycle matroids. On the other hand, we show that the more general DSFs share a variety of useful properties with decomposable functions. Namely, that they: (1) can leverage the vast amount of practical work on feature engineering that occurs in the machine learning community and its applications; (2) can operate on multi-modal data if the data can be featurized in the same space; (3) allow for training and testing on distinct sets since we can learn a function from the feature representation level on up, similar to the work in [92]; and (4) are useful for streaming [7, 83, 23] and parallel [107, 13, 14] optimization since functions can be evaluated without requiring knowledge of or access to the entire ground set. These advantages are made apparent in Section 2.

Interestingly, DSFs also share certain properties with deep neural networks (DNNs), which have become widely popular in the machine learning community. For example, DNNs with weights that are strictly non-negative correspond to a DSF. This suggests, as we show in Section 7.1, that it is possible to develop a learning framework over DSFs leveraging DNN learning frameworks. Unlike standard deep neural networks, which typically are trained either in classification or regression frameworks, however, learning submodularity often takes the form of trying to adjust the parameters so that a set of “summary” data sets are offered a high value. We therefore extend the max-margin learning framework of [140, 92] to apply to DSFs. Our approach can be seen as a max-margin learning approach for DNNs but restricted to DSFs.

We offer a list of applications for DSFs in machine learning and data science in Section 7.
2 Background and Motivation

Submodular functions are discrete set functions that have the property of diminishing returns. Given a finite size-\(n\) set of objects \(V\) (the ground set), where each \(v \in V\) is a distinct element. A valuation set function \(f : 2^V \to \mathbb{R}\) that returns a real value for any subset \(X \subseteq V\) is said to be submodular if for all \(X \subseteq Y\) and \(v \notin Y\) the following inequality holds: \(f(X \cup \{v\}) - f(X) \geq f(Y \cup \{v\}) - f(Y)\). This means that the incremental value (or gain) of adding another sample \(v\) to a subset decreases when the context in which \(v\) is considered grows from \(X\) to \(Y\). We can define the gain of \(v\) in the context of \(X\) as \(f(v|X) \triangleq f(X \cup \{v\}) - f(X)\). Thus, \(f\) is submodular if \(f(v|X) \geq f(v|Y)\). If the gain of \(v\) is identical for all different contexts i.e., \(f(v|X) = f(v|Y), \forall X,Y \subseteq V\) and \(\forall v \in V\), then the function is said to be modular. A function might also have the property of being normalized \((f(\emptyset) = 0)\) and monotone non-decreasing \((f(X) \leq f(Y)\) whenever \(X \subseteq Y\)). If \(f\) is a normalized monotone non-decreasing function, then it is often referred to as a polymatroid function [32, 31, 100] because it carries identical information to that of a polymatroidal polyhedron. If the negation of \(f\), \(-f\), is submodular, then \(f\) is called supermodular. If \(m\) is a normalized modular function, it can be written as a sum of singleton values \(m(X) = \sum_{x \in X} m(x)\) and, moreover, is seen simply as a vector \(m \in \mathbb{R}^V\).

A very simple example of a submodular function can be described using an urn containing a set of balls and a valuation function that counts the number of colors present in the urn. Such a function, therefore, measures only the diversity of ball colors in the urn, rather than ball quantity. We are motivated by applications where we wish to build models of information and diversity over data sets, in which case \(m\) is a ground set of data items. Each \(v \in V\), in such case, might be a distinct data sample — for example, either a word, n-gram, sentence, document, image, video, protein, genome, sensor reading, a machine learning system’s input-output training pair, or even a highly structured irregularly sized object such as a tree or a graph. It is also desirable for \(V\) to be a set of heterogeneous data objects, such where \(v_1 \in V\) may be an image and \(v_2 \in V\) may be a document.

There are many useful classes of submodular functions. One of the more widely used such function are those that, for the present purposes, we refer to a “graph based,” since they are parameterized by a weighted graph. Graph-based methods have a long history in many applications of machine learning and natural language processing (NLP), e.g., [103, 112, 2, 138, 144, 85, 96, 126, 159]. Work in this field is relevant to any graph-based submodular functions parameterized by a weighted graph \(G = (V, E, w)\), where \(V\) is a set of nodes (corresponding to the ground set), \(E\) is a set of edges, and \(w : E \to \mathbb{R}_+\) is a set of non-negative edge weights representing associations (e.g., affinity or similarity) between the corresponding elements. Graph-based submodular functions include the classic graph cut function \(f(X) = \sum_{x \in X, y \notin V \backslash X} w(x, y)\), but also the monotone graph cut function \(f(X) = \sum_{x \in X, y \notin V \backslash X} w(x, y)\), the saturated graph cut function [93] \(f(X) = \sum_{v \in V} \min(C_v(X), \alpha C_v(V))\) where \(\alpha \in (0, 1)\) is a hyperparameter and where \(C_v(X) = \sum_{x \in V} w(x, v)\). Another widely used graph-based function is the facility location function [106, 26, 113, 45]. This function, \(f(X) = \sum_{x \in X} \max_{v \in X} w(x, v)\). The maximization of which is related to the \(k\)-median problem [7, 75]. It is also useful and learn conic mixtures of graph based functions as done in [92].

An advantage of graph-based submodular functions is that they can be instantiated very easily, using only a similarity score between two objects \(v_1, v_2 \in V\) that does not require metricity or any property (such as non-negative definiteness of the associated matrix, required for using a determinantal point process (DPP) [51, 82, 48, 1, 49] other than non-negativity. A drawback of graph-based functions is that building a graph over \(n\) samples has complexity \(O(n^2)\) as has querying the function itself, something that does not scale to very large ground set sizes (although there are many approaches to more efficient sparse graph construction [25, 69, 25, 120, 153, 162] to improve upon this complexity). Moreover, it is difficult to add elements to \(V\) as it requires \(O(n)\) computation for each addition. For machine learning applications, moreover, it is difficult with these functions to train on a training set that may generalize to a test set [92].

3 Sums of Concave Composed with Modular Functions (SCMMs)

A class of submodular functions [141] used in machine learning are the so-called “decomposable functions.”. Given a set of non-negative modular functions \(m_i : V \to \mathbb{R}_+\), a corresponding set of non-negative monotone

\[^1\text{Lovász in 1980 uses the same definition, but also asked for integrality which Cunningham did not require.}\]
non-decreasing normalized (i.e., \( \phi(0) = 0 \)) concave functions \( \phi_i : [0, m_i(V)] \to \mathbb{R}_+ \), and a final normalized but otherwise arbitrary modular function \( m_\pm : V \to \mathbb{R} \), consider the class of functions \( g : 2^V \to \mathbb{R}_+ \) that take the following form:

\[
g(A) = \sum_i \phi_i(m_i(A)) + m_\pm(A) = \sum_i \phi_i \left( \sum_{a \in A} m_i(a) \right) + m_\pm(A).
\]

This class of functions is known to be submodular [47, 46, 141]. While such functions have been called “decomposable” in the past, in this work we will refer to this class of functions as “Sums of Concave over non-negative Modular plus Modular” (or SCMMs) in order to avoid confusion with the term “decomposable” used to describe certain graphical models [86, 53].

SCMMs have been shown to be quite flexible [141], being able to represent a surprisingly diverse set of functions. For example, consider the bipartite neighborhood function, which is defined using a bipartite graph \( G = (V, U, E, w) \) with \( E \subseteq V \times U \) being a set of edges between elements of \( V \) and \( U \), and where \( w : U \to \mathbb{R}_+ \) is a set of weights on \( U \). For any subset \( Y \subseteq U \) we define \( w(Y) = \sum_{y \in Y} w(y) \) as the sum of the weights of the elements \( Y \). The bipartite neighborhood function is then defined as \( g(X) = w(\Gamma(X)) \), where the neighbors function is defined as \( \Gamma(X) = \{ u \in U : \exists (x, u) \in E \text{ having } x \in X \} \subseteq U \) for \( X \subseteq V \). This can be easily written as an SCMM as follows: \( g(X) = \sum_{a \in A} w(u) \min(|X \cap \delta u|, 1) \) where \( \delta u \subseteq V \) are the neighbors of \( u \) in \( V \) — hence \( m_u(X) = |X \cap \delta u| \) is a modular function and \( \phi_u(\alpha) = \min(1, \alpha) \) is concave. When all the weights are unity, this is also equivalent to the set cover function \( g(X) = |\bigcup_{x \in X} \Gamma(x)| \) where the operation \( \min \) s.t. \( g(X) = |U| \) attempts to cover a set \( U \) by a small set of subsets \( \{ \Gamma(x) : x \in X \} \).

With such functions, it is possible to represent graph cut as follows: \( g(X) = f(X) + f(V \setminus X) - f(V) \), a sum of an SCMM and a complemented SCMM. It is shown in [72] that any SCMM can be represented with a graph cut function that might optionally utilize additional auxiliary variables that are first minimized over.

SCMMs can represent other functions as well, such as multiclass queuing system functions [63, 142], functions of the form \( f(A) = m_1(A) \phi(m_2(A)) \) where \( m_1, m_2 : V \to \mathbb{R}_+ \) are both non-negative modular functions, and \( \phi : \mathbb{R} \to \mathbb{R} \) is a non-increasing concave function. Another useful instance is the probabilistic coverage function [39] where we have a set of topics, indexed by \( i \), and \( V \) is a set of documents. The function, for topic \( u \), takes the form \( f_u(A) = 1 - \prod_{a \in A} (1 - p(u|a)) \) where \( p(u|a) \) is the probability of topic \( u \) for document \( a \) according to some model. This function can be written as \( f_u(A) = 1 - \exp(-\sum_{a \in A} \log(1/(1 - p(u|a)))) \) where \( \phi_u(\alpha) = 1 - \exp(-\alpha) \) is a concave function and \( m_u(A) = \sum_{a \in A} \log(1/(1 - p(u|a))) \) is modular. Hence, probabilistic coverage is an SCMM. Indeed, even the facility location function can be related to SCMMs. If in the facility location function we sum over a set of concepts \( U \) rather than the entire ground set \( V \) (which can be achieved, say by first clustering \( V \) into representatives \( U \)), the function takes the form \( g(A) = \sum_{a \in A} \max_{u \in U} w(a, u) \). A soft approximation to the max function (softmax) can be obtained as follows:

\[
\phi_{\text{softmax}(\gamma, w)}(A) \triangleq \frac{1}{\gamma} \log(\sum_{a \in A} \exp(\gamma w_u)).
\]

We have that \( \max_{a \in A} w_a = \lim_{\gamma \to \infty} \phi_{\text{softmax}(\gamma, w)}(A) \) and for any finite \( \gamma \), \( \phi_{\text{softmax}(\gamma, w)}(A) \) is a concave over modular function. Hence, a soft concept-based facility location function would take the form \( g_\gamma(A) = \sum_{u \in U} \phi_{\text{softmax}(\gamma, w_u)}(A) \) which is also an SCMM.

Equation (1) allows for a final arbitrary modular function \( m_\pm \) without which the function class would be strictly monotone non-decreasing and trivial to unconstrainedly minimize. Allowing an arbitrary modular function to apply at the end means the function class need not be monotone and hence finding the minimizing set is non-trivial. Because of their particular form, however, SCMMs yield efficient algorithms for fast minimization [141, 70, 117]. Moreover, it appears that there is little loss of generality in handling the non-monotonicity separately from the polymatroidality, as any non-monotone submodular function can easily be written as a sum of a totally normalized polymatroid function plus a modular function [31, 30]. To see

2In fact, the notion of decomposition used in [86, 53], the graphical models community, and related to the notion of the same name used in [31], can also be used to describe a form of decomposability of a submodular function in that the submodular function may be expressed as a sum of terms each one of which corresponds to a clique in a graph, and where the graph is triangulated, but where the terms need not be a concave composed with a modular function. Hence, without this switch of terminology, one reasonably could speak of “decomposable decomposable submodular functions.”
3.1 Feature Based Functions

A particularly useful way to view SCMMs for machine learning and data science applications is when data objects are embedded in a “feature” space indexed by a finite set $U$. Suppose we have a set of (possibly multi-modal) data objects $V$ each of which can be described by an embedding into feature space $\mathbb{R}_+^U$, where each $u \in U$ can be thought of as a possible feature, concept, or attribute of an object. Each object $v \in V$ is represented by a non-negative feature vector $m_U(v) = (m_{u_1}(v), m_{u_2}(v), \ldots, m_{u_{|U|}}(v)) \in \mathbb{R}_+^{|U|}$. Each feature $u \in U$ also has an associated normalized monotone non-decreasing concave function $\phi_u : [0, m_u(V)] \to \mathbb{R}_+$ and a non-negative importance weight $w_u$. These then yield the class of “feature based functions”

$$f(X) = \sum_{u \in U} w_u \phi_u(m_u(X)) + m_+(X)$$

(3)

where $m_u(X) = \sum_{x \in X} m_u(x)$. A feature based function then is an SCMM.

In a feature-based function, $m_u(v) \geq 0$ is a non-negative score that measures the degree of feature $u$ that exists in data object $v$ and the vector $m_U(v)$ is the entirety of the object’s representation in feature space. The quantity $m_u(X)$ measures the $u$-ness in a collection of objects $X$ that, when the concave function $\phi_u(\cdot)$ is applied, starts diminishing the contribution of this feature for that set of objects. The importance of each feature is given by the feature weight $w_u$. From the perspective of applications, $U$ can be any set of features.

As an example in NLP, let $V$ be a set of sentences. For $s \in V$ and $u \in U$, define $m_u(v)$ to be the count of n-gram feature $u$ in sentence $s$. For the sentence $s = \text{Whenever I visit New York City, I buy a New York City map.}$,
is identical to finding an 

Hence, the KL-divergence is merely a constant plus a difference of feature-based functions. Maximizing 

Let 

Next, create an 

maximizing this submodular function attempts to find a set that closely respect the feature weights. The concave function in the above is \( \phi(\alpha) = \log(\alpha) \) which is negative for \( \alpha < 1 \). We can rectify this situation by defining an extra object \( v' \notin V \) having \( m_u(v') = 1 \) for all \( u \). Then \( g(X|v') = \sum_{u \in U} p_u \log(1 + m_u(X)) \) is also a feature based function on \( V \).
The KL-divergence can be generalized in various ways, one of which is known as the $f$-divergence, or in particular the $\alpha$-divergence [137, 3]. Using the reparameterization $\alpha = 1 - 2\delta$ [74], the $\alpha$-divergence (or now $\delta$-divergence [165]) can be expressed as

$$D_\delta(p, q) = \frac{1}{\delta(1 - \delta)} (1 - \sum_{u \in U} p_u^\delta q_u^{1 - \delta}).$$

For $\delta \to 1$ we recover the standard KL-divergence above. For $\delta \in (0, 1)$ we see that the optimization problem $\text{min}_{X \subseteq V} m(X) \leq b \text{ } \text{ } D_\delta(p, \hat{p}(X))$ where $b$ is a budget constraint is the same as the constrained submodular maximization problem $\text{max}_{X \subseteq V} m(X) \leq g(X)$ where $g(X) = \sum_{u \in U} p_u^\delta (m_u(X))^{1 - \delta}$ is a feature-based function since $\phi_u(\alpha) = \alpha^{1 - \delta}$ is concave on $\alpha \in [0, 1]$ for $\delta \in (0, 1)$. Hence, any such constrained submodular maximization problem can be seen as a form of $\alpha$-divergence minimization.

Indeed, there are many useful concave functions one could employ in applications and that can achieve different forms of submodular function. Examples include the following: (1) the power functions, such as $\phi(\alpha) = \alpha^{1 - \delta}$ that we just encountered ($\delta = 1/2$ in Figures 1 (I)-(IV)); (2) the other non-saturating non-linearities such as $\phi(x) = \nu^{-1}(x)$ where $\nu(y) = y^3/3 + y$ [4] and the log functions $\phi_\gamma(\alpha) = \gamma \log(1 + \alpha/\gamma)$ with $\gamma > 0$ is a parameter; (3) the saturating functions such as $\phi(\alpha) = 1 - \exp(-\alpha)$, the logistic function $\phi(\alpha) = 1/(1 + \exp(-\alpha))$ and other “$s$”-shaped sigmoids (which are concave over the non-negative reals) such as the hyperbolic tangent, or $\phi(\alpha) = \left[1 - \frac{1}{\ln(b)} \ln \left(1 + \exp(-\alpha \ln(b))\right)\right]$ as used in [18, 78]; (4) and the hard truncation functions such as $\phi(\alpha) = \min(\alpha, \gamma)$ for some constant $\gamma$. There are also parameterized concave functions that get as close to the hard truncation functions as we wish, such as $\phi_{a,c}(x) = ((x^{-a} + c^{-a})^{-1}/a)$ where $a \geq -1$, and $c > 0$ are parameters — it is straightforward to show that $\phi_{-1,c}(x)$ is linear, that $\lim_{a \to \infty} \phi_{a,c}(x) = \min(x, c)$, and that for $-1 < a < \infty$ we have a form of soft min. Also recall the parameterized soft max mentioned above in relationship to the facility location function. In other cases, is useful for the concave function to be linear for a while before a soft or nonsaturating concave part kicks in, for example $\phi(\alpha) = \min(\sqrt{\alpha/\gamma}, \alpha/\gamma)$ for some constant $\gamma > 0$. These all can have their uses, depending on the application, and determine the nature of how the returns of a given feature $u \in U$ should diminish.

Feature based submodular functions, in particular, have been useful for tasks in speech recognition [155], machine translation [78], and computer vision [71].

We mention a final advantage of SCMMs is that they do not require the construction of a pairwise graph and therefore do not have quadratic cost as would, say a facility location function (e.g., $f(X) = \sum_{v \in V} \max_{x \in X} w_{vx}$), or any function based on pair-wise distances, all of which have cost $O(n^2)$ to evaluate. Feature functions have an evaluation cost of $O(n|U|)$, linear in the ground set $V$ size and therefore are more scalable to large data set sizes. Finally, unlike the facility location and other graph-based functions, feature-based functions do not require the use of the entire ground set for each evaluation and hence are appropriate for streaming algorithms [7, 23] where future ground elements are unavailable at the time one needs a function evaluation, as well as parallel submodular optimization [107, 13, 14]. For example, the vectors $m_U(v)$ for a newly encountered object $v$ can be computed on the fly (or in parallel) whenever the object $v$ is available and wherever it is located on a parallel machine.

## 4 Deep Submodular Functions

While feature-based submodular functions are indisputably useful, their weakness lies in that features themselves may not interact, although one feature $u'$ might be partially redundant with another feature $u''$. For example, when describing a sentence via its component n-grams features, higher-order n-grams always include lower-order n-grams, so some n-gram features can be partially redundant. For example, in a large collection of documents about “New York City”, it is likely there will be some instances of “Chicago,” so the feature functions for these two features should likely negatively covary. One way to reduce this redundancy is to subselect the features themselves, reducing them down to a subset that tends not to interact in any way. This can only work in limited cases, however, namely when the features themselves can be reduced to an “independent” set that looses no information about the data objects, and this only happens when redundancy is an all-or-nothing property (as in a matroid).

Most real-world features, however, involve partial redundancy. The presence of “New York City” shouldn’t completely remove the contributing of “Chicago”, rather it should only discount its contribution. A better
strategy, therefore, is to allow the feature scores to interact, say, when measuring redundancy at some higher-level concept of a “big city.”

Figure 1 offers a further pictorial example. Figure 1-(IV) shows that the most diverse set of size three is \{d, h, t\} since it has an even distribution over the set of features, square, triangle, circle. Suppose, however, the non-smooth shapes are seen to be partially redundant with each other, so that the presence of a square should discount, to some degree, the value of a triangle, but should not discount the value of a circle. The feature based function \(g(A) = \sum_{u \in \{\triangle, \square, \circ\}} \sqrt{m_u(A)}\) does not allow these three features to interact in any way to achieve this form of discounting. The contribution of “square” is measured combinatorially independently of “triangle” — feature-based functions therefore fail for features that themselves should be considered partially redundant. We can address this issue by using an additional level of concave composition

\[
g(A) = \sqrt{\sum_{u \in \{\triangle, \square, \circ\}} m_u(A)} + \sqrt{m_{\circ}(A)},
\]

where the nested square-root over the two features, square and triangle, allow them to interact and discount each other. Figure 1-(V) shows the new value of the formally maximum set \{d, h, f\} is no longer the maximum size-three set. Figure 1-(VI) shows the new maximum sized-three set, where the number of squares and circles together is roughly the same as the number of circles.

In general, to allow feature scores to interact and discount each other, we can utilize an additional “layer” of nested concave functions as follows:

\[
f(X) = \sum_{s \in S} \omega_s \phi_s \left( \sum_{u \in U} w_{s,u} \phi_u \left( m_u(X) \right) \right),
\]

where \(S\) is a set of meta-features, \(\omega_s\) is a meta-feature weight, \(\phi_s\) is a non-decreasing concave function associated with meta-feature \(s\), and \(w_{s,u}\) is now a meta-feature specific feature weight. With this construct, \(\phi_s\) assigns a discounted value to the set of features in \(U\), which can be used to represent feature redundancy. Interactions between the meta-features might be needed as well, and this can be done via meta-meta-features, and so on, resulting in a hierarchy of increasingly higher-level features. Such a hierarchy could correspond to semantic hierarchies for NLP applications (e.g., WordNet [105]), or a visual hierarchy in computer vision (e.g., ImageNet [34]). Alternatively, in the spirit of modern big-data efforts in deep learning, such a hierarchy could be learnt automatically from data.

We propose a new class of submodular functions that we call deep submodular functions (DSFs). They may make use of a finite-length series of disjoint sets (see Figure 2-(a)): \(V = V^{(0)}\), which is the function’s ground set, and additional sets \(V^{(1)}, V^{(2)}, \ldots, V^{(K)}\). \(U = V^{(1)}\) can be seen as a set of “features”, \(V^{(2)}\) as a set of meta-features, \(V^{(3)}\) as a set of meta-meta-features, etc. up to \(V^{(K)}\). The size of \(V^{(i)}\) is \(d^i = |V^{(i)}|\). Two successive sets (or “layers”) \(i - 1\) and \(i\) are connected by a matrix \(w^{(i)} \in \mathbb{R}_{+}^{d^{i-1} \times d^{i-1}}\), for \(i \in \{1, \ldots, K\}\). Hence, rows of \(w^{(i)}\) are indexed by elements of \(V^{(i)}\) and columns of \(w^{(i)}\) are indexed by elements of \(V^{(i-1)}\). Given \(v^i \in V^{(i)}\), define \(w^{(i)}_{v^i}\) to be the row of \(w^{(i)}\) corresponding to element \(v^i\), and \(w^{(i)}_{v^i}(v^{i-1})\) is the element
of matrix \(w^{(i)}\) at row \(v^i\) and column \(v^{i-1}\). We may think of \(w^{(i)}_{v^i} : V^{(i-1)} \rightarrow \mathbb{R}_+\) as a modular function defined on set \(V^{(i-1)}\). Thus, this matrix contains \(d^i\) such modular functions. Further, let \(\phi_v : \mathbb{R}_+ \rightarrow \mathbb{R}_+\) be a non-negative non-decreasing concave function. Then, a \(K\)-layer DSF \(f : 2^V \rightarrow \mathbb{R}_+\) can be expressed as follows, for any \(A \subseteq V\),
\[
f(A) = \tilde{f}(A) + m_\pm(A) \tag{9}
\]
where,
\[
\tilde{f}(A) = \phi_v \left( \sum_{v^{K-1} \in V^{(K-1)}} w^{(K)}_{v^{K-1}}(v_{K-1}) \phi_{u^{K-1}} \left( \ldots \sum_{v^2 \in V^{(2)}} w^{(3)}_{v^2}(v^2) \phi_{u^2} \left( \sum_{v^1 \in V^{(1)}} w^{(2)}_{v^1}(v^1) \phi_{u^1} \left( \sum_{a \in A} w^{(1)}_{v^1}(a) \right) \right) \right) \right),
\]
and where \(m_\pm : V \rightarrow \mathbb{R}\) is an arbitrary modular function. Equation (9) defines a class of submodular functions. Submodularity follows since a composition of a monotone non-decreasing function \(h\) and a monotone non-decreasing concave function \(\phi\) (\(g(v) = \phi(h(v))\)) is submodular (Theorem 1 in [31, 30] and repeated, with proof, in Theorem 5.4) — a DSF is submodular via recursive application and since submodularity is closed under conic combinations.

### 4.1 Recursively Defined DSFs

A slightly more general way to define a DSF and that is useful for the theorems below uses recursion. This section also defines the notation that will be often used later in the paper.

We are given a directed acyclic graph (DAG) \(G = (V, E)\) where for any given node \(v \in V\), we say \(pa(v) \subset V\) are the parents of (or vertices pointing towards) \(v\). A given size \(n\) subset of nodes \(V \subset V\) corresponds to the ground set of a submodular function and for any \(v \in V\), \(pa(v) = \emptyset\). A unique "root" node \(x \in V \setminus V\) has the distinction that \(x \notin pa(q)\) for any \(q \in V\). Given a non-ground node \(v \in V \setminus V\), we define the concave function \(\psi_v : \mathbb{R}^V \rightarrow \mathbb{R}_+\) where
\[
\psi_v(x) = \phi_x(\varphi_v(x)), \tag{11a}
\]
and
\[
\varphi_v(x) = \sum_{u \in pa(v) \setminus V} w_{uv} \psi_u(x) + \langle m_v, x \rangle. \tag{11b}
\]

In the above, \(\phi_v : \mathbb{R}_+ \rightarrow \mathbb{R}_+\) is a normalized non-decreasing univariate concave function, \(w_{vu} \in \mathbb{R}_+\) is a non-negative weight indicating the relative importance of \(\psi_u\) to \(\varphi_v\), and \(m_v : \mathbb{R}^{pa(v) \cap V} \rightarrow \mathbb{R}_+\) is a non-negative linear function that evaluates as \(\langle m_v, x \rangle = \sum_{u \in pa(v) \setminus V} m_v(u)x(u)\). In other words, \(\langle m_v, x \rangle\) is a sparse dot-product over ground elements \(pa(v) \cap V\). There is no additional additive bias constant added to the end of Equation (11b) as this is assumed to be part of \(\phi_v\) (as a shift) if needed (alternatively, for one of the \(u \in pa(V) \setminus V\), we can set \(\psi_u(x) = 1\) as a constant, and the bias may be specified by a weight, as is occasionally done when specifying neural networks). The base case, where \(pa(v) \subseteq V\) therefore has \(\psi_v(x) = \phi_v(\langle m_v, x \rangle)\), so \(\psi_v(1_A)\) is a concave composed with a modular function. The notation \(1_A\) indicates the characteristic vector of set \(A\), meaning \(1_A(v) = 1\) if \(v \in A\) and is otherwise zero.

A general DSF is defined as follows: for all \(A \subseteq V\), \(f(A) = \psi_v(1_A) + m_\pm(A)\), where \(m_\pm : V \rightarrow \mathbb{R}\) is an arbitrary modular function (i.e., it may include positive and negative elements). For all \(v \in V\), we also for convenience, define \(g_v(A) = \psi_v(1_A)\). To be able to treat all \(v \in V\) similarly, we say, for \(v \in V\), that \(pa(v) = \emptyset\), and use the identity \(\phi_v(a) = a\) for \(a \in \mathbb{R}\), and set \(m_v = 1_v\), so that \(\psi_v(x) = \varphi_v(x) = x(v)\) and \(g_v(A) = 1_{v \in A}\) which is a modular function on \(V\).

By convention, we say that a zero-layer DSF function is an arbitrary modular function, a one-layer DSF is an SCMM, and a two-layer DSF is, as we will soon see, something different. By DSF\(_k\), we mean the family of DSFs with \(k\) layers.

As mentioned above, from the perspective of defining a submodular function, there is no loss of generality by adding the final modular function \(m_\pm\) to a polymatroid function [31, 30]. The degree to which DSFs
comprise a subclass of submodular functions corresponds to the degree to which \( g_s \) comprise a subclass of all polymatroid functions.

The recursive form of DSF is more convenient than the layered approach mentioned above which, in the current form, would partition \( V = \{ V^{(0)}, V^{(1)}, \ldots, V^{(K)} \} \) into layers, and where for any \( v \in V^{(i)} \), \( \text{pa}(v) \subseteq V^{(i-1)} \). Figure 2-(a) corresponds to a layered graph \( G = (V, E) \) where \( r = v_1^0 \) and \( V = \{ v_0^0, v_0^1, \ldots, v_0^0 \} \). Figure 2-(b) uses the same partitioning but where units are allowed to skip by more than one layer at a time. More generally, we can order the vertices in \( V \) with order \( \sigma \) so that \( \{ \sigma_1, \sigma_2, \ldots, \sigma_n \} = V \) where \( n = |V| \), \( \sigma_m = v = v^K \) where \( m = |V| \) and where \( \sigma_i \in \text{pa}(\sigma_j) \) iff \( i < j \). This allows an arbitrary pattern of skipping while maintaining submodularity. The additional linear function in Equation (11b) is strictly not necessary (e.g., there could be paths of linearity along subsets of the \( \phi, v \in A \) for some \( A \subseteq V \) thereby achieving the same result) but we include it to stress that at each layer there may be a modular function and a bias.

### 4.2 DSFs: Practical Benefits and Relation to Deep Neural Networks

The layered definition in Equation (9) is reminiscent of feed-forward deep neural networks (DNNs) owing to its multi-layered architecture. Interestingly, if one restricts the weights of a DNN at every layer to be non-negative, then for many standard hidden-unit activation functions the DNN constitutes a submodular function when given Boolean input vectors. The result follows for any activation function that is monotone non-decreasing concave for non-negative reals, such as the sigmoid, the hyperbolic tangent, and the rectified linear functions. In the rectified linear case, however, the entire network would be linear so the model becomes interesting only with hidden activations that are strictly concave (since the weights can be arbitrarily scaled, perhaps \( \phi(x) = \min(x, 1) \) is a reasonable concave analogy in a DSF to the rectified linear function in a DNN).

More importantly, this suggests that DSFs can be trained in a fashion similar to DNNs — specifically, training DSFs and can take advantage of the many successful training techniques and software libraries for training DNNs (many of the toolkits make it easy to project weights into the positive orthant). Further discussion on this point is given in Section 7.1. The recursive definition of DSFs, in Equation (11) is useful for the analysis in Section 5.

DSFs should be useful for many applications in machine learning. First, they retain the advantages of SCMMs in that they require neither \( O(n^2) \) computation nor access to the entire ground set for a set evaluation. The underlying DSF computation is matrix-vector multiplication that, like DNNs, can be performed very quickly using modern GPU computing. Hence, DSFs can be both fast, and useful for parallel and/or streaming applications. Second, DSFs allow for a nested hierarchy of features, similar to advantages a deep model has over a shallow model. For example, a one-layer DSF must construct a valuation over a set of objects from a large number of low-level features which can lead to fewer opportunities for feature sharing while a deeper network fosters distributed representations, also analogous to DNNs [15, 16]. It can be argued that a deep neural network is more efficient, in terms of the number of possible functions represented per weight, than a shallow neural network and perhaps DSFs share this advantage. Hence, even if the DSF and SCMM families were to be found to be same (but that Theorem 6.4 shows to be false), there could be advantages to applications and learning paradigms thanks to this natural hierarchical decomposition of concepts.

DSFs have been used occasionally in some applications. In one instance [95], a square root was applied to a subset of the right hand nodes in a bipartite neighborhood function in order to offer reduced cost for these nodes being indirectly selected in the graph. In [155] a two-layer DSF was used to introduce higher-level interaction between features, an act that yielded benefits in speech data summarization. Lastly, laminar matroid rank functions, which are instances of DSFs as shown in Section 5.3, have been used to show worst case performance of various constrained submodular minimization problems [52, 145, 66].

### 5 Relevant Properties and Special Cases

DSFs represent a family that, at the very least, contain the family of SCMMs. Above, we argued intuitively that DSFs might extend SCMMs as they allow components themselves to directly interact, and the interactions may propagate up a many-layered hierarchy. In this section, we start off (in Section 5.1) discussing preliminaries regarding concave functions. Section 5.2 then covers specific properties of the multivariate concave function associated with a DSF, in particular the antitone gradient superdifferential property which
is a sufficient condition for submodularity. This section also compares this condition with the negativity of the off-diagonal Hessian matrix condition for submodular functions. Section 5.3 discusses matroid rank special cases, including the laminar matroid rank function which can be seen, in the light of this paper, as a form of deep matroid rank. This section also discusses special cases of the results shown later in the paper, in particular, that: (1) cycle matroid rank functions cannot represent all partition matroid rank functions; (2) laminar matroid rank functions strictly generalize partition matroid rank functions; (3) laminar matroid rank functions cannot express all cycle matroid rank functions; (4) DSFs generalize laminar matroid rank functions; and (5) SCMMs generalize partition matroid rank functions. Lastly, section 5.4 introduces various analysis tools (in particular the “surplus”) that are used later in the paper.

### 5.1 Properties of Concave and Submodular Functions

Many of the results in the sections below rely on a number of properties of concave functions. Since we wish to consider non-differentiable concave functions, the theorems below consider this more general case where we may assume only that the concave functions have superdifferentials. It is, in general, more work to show that the properties of concave functions hold in this non-differential case, but since there seem to be no consolidated published proofs of these properties, we offer them here in full.

Let \( \phi : \mathbb{R} \rightarrow \mathbb{R} \) be a normalized \((\phi(0) = 0)\) monotone non-decreasing concave function. In any such function, there may be an initial linear part where \( \phi(x) = \gamma x \) for \( x \in [0, \alpha] \) where \( \gamma > 0 \) and where \( \alpha \geq 0 \) is the largest point where \( \phi \) is still linear. Larger than \( \alpha \), there may be a middle part consisting of a series of concave curves and line segments all situated to ensure concavity. Larger than this, there finally might be a saturation point where \( \phi(x) = c \) for all \( x \geq \alpha_{\text{sat}} \), where \( c, \alpha_{\text{sat}} \in \mathbb{R}_+ \cup \{\infty\} \). The middle region \( (x \in [\alpha_{\text{lin}}, \alpha_{\text{sat}}]) \) might or might not be smooth. It is useful sometimes in applications (e.g., \cite{71}) to formulate submodular functions from concave functions that have an initial linear part followed by either a saturation or by a smooth concave part.

**Definition 5.1 (Superdifferential).** Let \( \phi : \mathbb{R}^n \rightarrow \mathbb{R} \) be a concave function. The superdifferential of \( \phi \) at \( x \) is the set of vectors defined as follows:

\[
\partial \phi(x) = \{ s \in \mathbb{R}^n : f(y) - f(x) \leq \langle s, y - x \rangle, \forall y \in \mathbb{R}^n \} \tag{12}
\]

The superdifferential of a concave function is guaranteed always to exist \cite{128, 129, 60, 114}. When \( \phi \) is differentiable at \( x \), the superdifferential corresponds to the gradient, so that \( \partial \phi(x) = \{ \nabla \phi(x) \} \) and otherwise members of \( \partial \phi(x) \) are called subgradients. In general, we have the following:

**Lemma 5.2.** The superdifferential of a concave function is a monotone operator, i.e.,

\[
\langle u - v, x - y \rangle \leq 0, \forall x, y \in \mathbb{R}^n, u \in \partial \phi(x), v \in \partial \phi(y) \tag{13}
\]

**Proof.** We have that

\[
f(y) \leq f(x) + \langle u, y - x \rangle, \text{ and } f(x) \leq f(y) + \langle v, x - y \rangle \tag{14}
\]

Adding the two inequalities yields monotonicity.

This means in particular that, in the one-dimensional case when \( n = 1 \), if \( x \leq y \) then for any \( u \in \partial \phi(x) \) and any \( v \in \partial \phi(y) \), we must have \( u \geq v \). In the below, we offer a number of properties of concave superdifferentials in the 1D case. While statements of these results are intuitively clear, the authors were unable to find published proofs, so they are also included herein.

**Theorem 5.3.** Let \( \phi : \mathbb{R} \rightarrow \mathbb{R} \) be a continuous function. Then \( \phi \) is concave if and only if for all \( a, b \in \mathbb{R} \) with \( a \leq b \), and \( \Delta \in \mathbb{R}_+ \), we have that

\[
\phi(a + \Delta) - \phi(a) \geq \phi(b + \Delta) - \phi(b) \tag{15}
\]

Also, \( \phi \) is monotone non-decreasing concave if and only if for all \( a, b \in \mathbb{R} \) with \( a \leq b \), and \( \Delta, \epsilon \in \mathbb{R}_+ \), we have that

\[
\phi(a + \Delta + \epsilon) - \phi(a) \geq \phi(b + \Delta) - \phi(b) \tag{16}
\]
Proof. The result is vacuous if \( a = b \), or \( \Delta = 0 \) so assume \( a < b \) and \( \Delta > 0 \).

If part: Assume Equation (15) is true and consider
\[
\frac{\phi(a + \Delta) - \phi(a)}{\Delta} \geq \frac{\phi(b + \Delta) - \phi(b)}{\Delta}
\] (17)

If \( \phi \) is differentiable at \( a \) and \( b \), then taking \( \Delta \to 0 \) gives us \( \phi'(a) \geq \phi'(b) \) for all \( a \leq b \), and this is a sufficient condition for concavity (see Nesterov 2.13, page 54, [114]). If \( \phi \) is not differentiable at either \( a \) or \( b \), we resort to its continuity. A function is concave if and only if it is continuous and midpoint concave [116] (or midconcave [127]), defined as for any \( x, y \in \mathbb{R} \), \( f((x+y)/2) \geq (f(x) + f(y))/2 \). This condition is immediate from Equation (15) by setting \( x = a, y = b + \Delta \), and \( b = a + \Delta = (x+y)/2 \).

Only if part: Assume \( \phi \) is concave and \( a < b \) and \( \Delta > 0 \) are given. If \( \phi \) is differentiable, then by the mean value theorem, there exists an \( a^+ \) with \( a \leq a^+ \leq a + \Delta \) and an \( b^+ \) with \( b \leq b^+ \leq b + \Delta \) where
\[
\phi'(a^+) = \frac{\phi(a + \Delta) - \phi(a)}{\Delta}
\]
and
\[
\phi'(b^+) = \frac{\phi(b + \Delta) - \phi(b)}{\Delta}
\] (19)

If \( a + \Delta \leq b \) then \( a^+ \leq b^+ \) and hence \( \phi'(a^+) \geq \phi'(b^+) \) by concavity (Nesterov) which immediately gives \( \phi(a + \Delta) - \phi(a) \geq \phi(b + \Delta) - \phi(b) \). If \( \phi \) is not differentiable at either \( a \) or \( b \), then consider \( d_a \in \partial \phi(a) \) and \( d_b \in \partial \phi(b) \), so that \( \forall y_a, y_b, \phi(y_a) \leq \phi(a) + \langle d_a, y_a - a \rangle \) and \( \phi(y_b) \leq \phi(b) + \langle d_b, y_b - b \rangle \). Taking \( y_a = a + \Delta \) and \( y_b = b + \Delta \) gives \( (\phi(a + \Delta) - \phi(a))/\Delta = d_a \geq d_b = (\phi(b + \Delta) - \phi(b))/\Delta \) which follows from the monotonicity of the superdifferential operator.

If \( a + \Delta > b \) then \( a < b < a + \Delta < b + \Delta \). Again when \( \phi \) is differentiable, by the mean value theorem, there exists \( a_b^+ \) with \( a \leq a_b^+ \leq b \) and \( a_+^{\Delta} \) with \( a + \Delta \leq a_+^{\Delta} \leq b + \Delta \) with
\[
\phi'(a_b^+) = \frac{\phi(b) - \phi(a)}{b - a}
\]
and
\[
\phi'(a_+^{\Delta}) = \frac{\phi(b + \Delta) - \phi(a + \Delta)}{b - a},
\] (21)
and since \( a_b^+ < a_+^{\Delta} \), \( \phi'(a_b^+) \geq \phi'(a_+^{\Delta}) \). This immediately gives \( \phi(b) - \phi(a) \geq \phi(b + \Delta) - \phi(a + \Delta) \) or \( \phi(a + \Delta) - \phi(a) \geq \phi(b + \Delta) - \phi(b) \). If \( \phi \) is not differentiable, then taking supergradients \( d_a \in \partial \phi(a) \) and \( d_{a+\Delta} \in \partial \phi(a + \Delta) \) again gives the result.

The second part of the theorem is immediate if we take \( a = b \), and define \( \delta = a + \Delta \) leading to \( \phi(\delta + \epsilon) \geq \phi(\delta) \), i.e., monotonicity.

The above proof considers the smooth and non-smooth varieties separately where the non-smooth case utilizes only the existence of the superdifferential of a concave function. Since the superdifferential always exists for a concave function, smooth or otherwise, in the below we consider only the most general case where we assume only a superdifferential exists. As a result, the proofs are a bit more involved, but when constructing DSFs and considering the resultant submodular families in Section 6, we wish to allow for the most general class concave functions.

We next restate Theorem 1 from [93] but also provide a proof which was missing.

**Theorem 5.4.** Suppose that \( h : 2^V \to \mathbb{R} \) is a monotone non-decreasing submodular function and \( \phi \) is a monotone non-decreasing concave function. Then \( g(A) = \phi(h(A)) \) is monotone non-decreasing submodular.

**Proof.** Consider any \( A \subseteq B \subseteq V \) and \( v \notin B \). Define quantities \( a, b, \Delta, \epsilon \) so that: \( a = h(A) \leq b = h(B) \), \( a + \Delta + \epsilon = h(A + v) \), and \( b + \Delta = h(B + v) \). I.e., \( h(v \mid A) = \Delta + \epsilon \leq h(v \mid B) = \Delta \). Then we have
\[
\phi(a + \Delta + \epsilon) - \phi(a) \geq \phi(b + \Delta) - \phi(b)
\] (22)
or
\[
\phi(h(A + v)) - \phi(h(A)) \geq \phi(h(B + v)) - \phi(h(B)).
\]  
(23)

The slope of the linear interpolation between two points on a concave function puts a connecting relationship on the corresponding superdifferentials at each of the two points, as the following result shows.

**Lemma 5.5.** Given a concave function \( \phi : \mathbb{R} \to \mathbb{R} \) and two points \( a, b \) with \( a < b \) that define the value \( d_{ab} = (\phi(b) - \phi(a))/(b - a) \). Then \( \min_{d \in \partial \phi(a)} d > d_{ab} \) if and only if \( \max_{d \in \partial \phi(b)} d < d_{ab} \).

**Proof.** From the monotonicity of the supergradient [60, 114], we always have
\[
\frac{\partial \phi}{\partial \phi(a)} \leq \min_{d \in \partial \phi(a)} d \geq d_{ab} \geq \max_{d \in \partial \phi(b)} d \leq \frac{\partial \phi}{\partial \phi(b)} \tag{24}
\]

since otherwise, say if \( d_{a}^{\min} < d_{ab} \), then \( \phi(a) + d_{a}^{\min}(b - a) < \phi(a) + d_{ab}(b - a) = \phi(b) \) which contradicts \( d_a^{\min} \) being a supergradient. We must show that the inequalities in Equation (24) can be only simultaneously strict. Let \( d_a^{\min} \) be given such that \( d_a^{\min} > d_{ab} \), and suppose that \( d_b^{\max} = d_{ab} \). Then
\[
\phi(y) \leq \phi(b) + d_b^{\max}(y - b)
= \phi(b) + d_b^{\max}(y - a + a - b)
= \phi(b) + d_b^{\max}(a - b) + d_b^{\max}(y - a)
= \phi(a) + d_b^{\max}(y - a)
\]

and hence we have found a supergradient \( d_b^{\max} \in \partial \phi(a) \) with \( d_a^{\min} > d_b^{\max} \) contradicting the minimality of \( d_a^{\min} \). Hence, we must have \( d_b^{\max} < d_{ab} \). A similar argument shows that \( d_b^{\max} < d_{ab} \) and \( d_a^{\min} = d_{ab} \) leads to a contradiction of the maximality of \( d_b^{\max} \).

The next result identifies a condition that, if true, tells us about the extent of the initial linear region of a monotone non-decreasing concave function.

**Theorem 5.6.** Given a monotone non-decreasing concave function \( \phi : \mathbb{R} \to \mathbb{R} \) that is normalized (\( \phi(0) = 0 \)) and any \( a, b \in \mathbb{R}_+ \) with \( 0 < a \leq b \). Then \( \phi(a + b) = \phi(a) + \phi(b) \), if and only if \( \phi(x) \) is linear in the region from \( 0 \) to \( a + b \) (that is, there exists \( \gamma \in \mathbb{R} \) with \( \phi(x) = \gamma x \) for \( x \in [0, a + b] \)).

**Proof.** If case: immediate.

Only if case: Any violations of the following inequalities would violate the superdifferential property of \( \partial \phi(y) \) at \( 0, a, b, \) or \( a + b \):
\[
\min_{d \in \partial \phi(0)} d \geq \frac{\phi(a)}{a}, \quad \max_{d \in \partial \phi(a)} d \leq \frac{\phi(a)}{a}, \tag{29}
\]
\[
\min_{d \in \partial \phi(a)} d \geq \frac{\phi(b) - \phi(a)}{b - a}, \quad \max_{d \in \partial \phi(b)} d \leq \frac{\phi(b) - \phi(a)}{b - a}, \tag{30}
\]
\[
\min_{d \in \partial \phi(b)} d \geq \frac{\phi(a + b) - \phi(b)}{(a + b) - a} = \frac{\phi(a)}{a}, \quad \max_{d \in \partial \phi(a + b)} d \leq \frac{\phi(a)}{a}. \tag{31}
\]

This leads to the series of inequalities:
\[
\min_{d \in \partial \phi(0)} d \geq \frac{(a)}{a} \geq \max_{d \in \partial \phi(a)} d \geq \min_{d \in \partial \phi(a)} d \geq \frac{\phi(b) - \phi(a)}{b - a} \geq \max_{d \in \partial \phi(b)} d \geq \min_{d \in \partial \phi(b)} d \tag{32}
\]
\[
\geq \min_{d \in \partial \phi(b)} d \geq \frac{\phi(a)/a}{\max_{d \in \partial \phi(a+b)} d} \geq \frac{\phi(a)/a}{\max_{d \in \partial \phi(a+b)} d} \tag{33}
\]

From Lemma 5.5, if (a) is strict, then so is (b), leading to the contradiction \( \phi(a)/a > \phi(a)/a \). Also from Lemma 5.5, if (d) is strict, then so is (c), leading to the same contradiction. Hence, all inequalities are
Hence, for all \( y \in [0, a + b] \), we have \( \partial \phi(y) = \{ \phi(a)/a \} \), meaning that \( \phi \) is linear in this region with \( \gamma = \phi(a)/a = \phi(b)/b = \phi(a + b)/(a + b) \).

It is known that any normalized submodular function is subadditive, in that for any \( A \subseteq V \), \( \sum_{a \in A} f(a) \geq f(A) \). A similar property is true of normalized monotone non-decreasing concave functions.

**Theorem 5.7** (Subadditivity). Given a normalized monotone non-decreasing concave function \( \phi \), a set of non-negative points \( \{ x_i \}_{i=1}^\ell \), \( x_i \in \mathbb{R}_+ \), then we have

\[
\sum_i \phi(x_i) \geq \phi(\sum_i x_i)
\]

and where the inequality is strict if and only if \( \sum_i x_i \) is past any linear part of \( \phi \).

**Proof.** It is sufficient to show that it is true for \( x_1 \leq \cdots \leq x_{\ell-1} \leq x_\ell \) that

\[
\phi(x_1 + \cdots + x_{\ell-1} + x_\ell) \geq \phi(x_1 + \cdots + x_{\ell-1}) + \phi(x_\ell)
\]

then apply it inductively with \( x_1 \leq \cdots \leq x_{\ell-2} \leq x_{\ell-1} \). Hence, we only need to show that \( \phi(x_1) + \phi(x_2) \geq \phi(x_1 + x_2) \), and we get this immediately setting \( a = 0, \Delta = x_1, b = x_2 \) in Equation (15).

The strictness part follows from Theorem 5.6, where it states that equality in \( \phi(x_1 + \cdots + x_{\ell-1}) + \phi(x_\ell) = \phi(\sum_i x_i) \) holds if and only if \( \phi \) is linear from 0 through \( x_1 + \cdots + x_{\ell-1} + x_\ell = \sum_i x_i \).

The next result shows that when an SCMM has only one term, the addition of the final modular function \( m_\pm \) extends the family. We in show that this is the case, even when \( m_\pm \) is non-negative.

**Theorem 5.8.** The family of an SCMM with one concave over modular term is enlarged by an additional modular term \( m_\pm \).

**Proof.** Consider a three-element ground set \( V = \{ a, b, c \} \) and a function \( g \),

\[
g(A) = \min(|A|, 1) + 1_{c \in A},
\]

thus \( g \) is monotone non-decreasing. Suppose \( g(A) = \phi(m(A)) \) for some non-negative modular function \( m \) and normalized non-decreasing concave function \( \phi \). Then by Equation (24), we have:

\[
\min_{d \in \partial \phi(m(a))} d \geq \frac{\phi(m(a,b)) - \phi(m(a))}{m(a,b) - m(a)} = \max_{d \in \partial \phi(m(a,b))} d \geq 0
\]

where the (iii) follows since \( \phi \) is monotone. Hence, (ii) is an equality and by Lemma 5.5 so is (i). Hence 0 \( \in \partial \phi(m(a)) \). Then we have that \( \phi(y) \leq \phi(m(a,b)) + (y - m(a,b)) \). This means that \( \phi(m(a,b,c)) \leq \phi(m(a,b),c) = 1 < 2 = g(a,b,c) \), a contradiction.

An immediate corollary is that SCMMs are a larger class of submodular functions than just one concave over modular function. All SCMMs, however, can be represented as a sum of modular truncations as the following lemma states:

**Lemma 5.9** (Sums of Modular Truncations [141]). If \( f \) is an SCMM, then \( f \) may be written as \( f(A) = \sum_i \min(m_i(A), \beta_i) + m_\pm(A) \) where for all \( i \), \( m_i \) is a non-negative modular function, \( \beta_i \geq 0 \) is a non-negative constant, and where the sum is over a finite number of terms.

Truncating modular function is important, as it is not sufficient to truncate only cardinality functions. In other words, SCMMs also generalize the family of weighted cardinality truncations, as the next result shows.
Lemma 5.10 (Sums of Weighted Cardinality Truncations). We define the class of sums of weighted cardinality truncations as

\[ G = \left\{ g : \forall A, g(A) = \sum_{B \subseteq V} \sum_{i=1}^{|B|-1} \alpha_{B,i} \min(|A \cap B|, i), \quad \forall B, i, \alpha_{B,i} \geq 0 \right\}. \]

Then there exists an \( f \in \text{SCMM} \text{ that is not in } G. \)

Lemma 5.10 is proven in Appendix B.

5.2 Antitone Maps and Superdifferentials

Thanks to concave composition closure rules [19], the root function \( \psi(x) : \mathbb{R}^n \to \mathbb{R} \) in Eqn. (11) is a monotone non-decreasing multivariate concave function that, by the concave-submodular composition rule (Theorem 5.4) yields a submodular function \( \psi(1_A) \). It is widely known that any univariate concave function composed with non-negative modular functions yields a submodular function. However, given an arbitrary multivariate concave function this is not the case. Consider, for example, any concave function \( \psi \) defined as

\[ \psi((0,0)) = \psi(1,1) = 1, \quad \psi(0,1) = \psi(1,0) = 0. \]

Then \( f(A) = \psi(1_A) \) is not submodular, and hence the guarantee of submodularity when composing a concave with a linear function does not extend to dimensions higher than one. In this section, we discuss a limited form of such a generalization, one that ensures submodularity and that, moreover, does not even always rely on concavity in higher dimensions. Here and below, for \( x, y \in \mathbb{R}^V \), then \( x \leq y \iff x(v) \leq y(v), \forall v \in V \).

Definition 5.11. A concave function is said to have an antitone superdifferential if for all \( x \leq y \) we have that \( h_x \geq h_y \) for all \( h_x \in \partial \psi(x) \) and \( h_y \in \partial \psi(y) \).

The antitone superdifferential is an apparently straightforward multidimensional generalization of a defining characteristic of univariate concave functions. Theorem 5.12 below generalizes Theorem 5.4 when \( k = 1 \) — this is because \( \phi : \mathbb{R} \to \mathbb{R} \) being concave is, in the univariate case, synonymous with it having an antitone superdifferential (which is synonymous with monotone supergradients [60, 114]).

Theorem 5.12. Let \( \psi : \mathbb{R}^k \to \mathbb{R} \) be a monotone non-decreasing concave function and let \( \bar{g} : 2^V \to \mathbb{R}^k \) be a vector of polymatroid functions, where \( \bar{g}(A) = (g_1(A), g_2(A), \ldots, g_k(A)) \). Then if \( \psi \) has an antitone superdifferential, then the set function \( f : 2^V \to \mathbb{R} \) defined as \( f(A) = \psi(\bar{g}(A)) \) for all \( A \subseteq V \) is submodular.

Proof. Given two points \( x, y \in \mathbb{R}^n \) with \( x \leq y \), then the fundamental theorem of calculus for line integrals states that for any smooth relative path \( p \) from \( x \) to \( y \), the integral through the vector field \( \nabla \psi(x) \) yields

\[ \psi(y) - \psi(x) = \int_0^1 \nabla \psi(x + t(y-x)) \cdot dp(t) \]

If \( \psi \) is not differentiable, we may assume, with a slight abuse of notation, that \( \nabla \psi(x) \) is any gradient map for all \( x \in \mathbb{R}^n \) (i.e., \( \nabla \psi(x) \) maps from \( x \) to some element within \( \partial \psi(x) \)). Given an arbitrary \( A \subseteq B \) and \( v \not\in B \), and let \( p(t) \) be any relative and parametric curve from a point \( \bar{g}(A) \in \mathbb{R}^k \) when \( t = 0 \) to a point \( \bar{g}(A + v) \in \mathbb{R}^k \) when \( t = 1 \). Hence, \( \bar{g}(A) + p(0) = \bar{g}(A) \) and \( \bar{g}(A) + p(1) = \bar{g}(A + v) \). Since \( \bar{g} \) is a vector of polymatroid functions, we have \( \bar{g}(A) \leq \bar{g}(B) \) and \( \bar{g}(A) \leq \bar{g}(A + v) \), and hence, the path \( p(t) \) can be taken to be monotone, so that \( 0 \leq p(t_1) \leq p(t_2) \) whenever \( 0 \leq t_1 \leq t_2 \leq 1 \). Other than monotonicity, the path may be arbitrary. By monotonicity and submodularity, \( 0 \leq \bar{g}(B + v) - \bar{g}(B) \leq \bar{g}(A + v) - \bar{g}(A) \), and hence we may choose the relative path that starts at 0, and at some point \( t' \in (0, 1) \), goes through the point \( p(t') = \bar{g}(B + v) - \bar{g}(B) \), and ends up at \( p(1) = \bar{g}(A + v) - \bar{g}(A) \). Then,

\[ f(A + v) - f(A) = \psi(\bar{g}(A + v)) - \psi(\bar{g}(A)) = \int_0^1 \nabla \psi(\bar{g}(A) + p(t)) \cdot dp(t) \]

\[ \geq \int_0^{t'} \nabla \psi(\bar{g}(A) + p(t)) \cdot dp(t) \geq \int_0^{t'} \nabla \psi(\bar{g}(B) + p(t)) \cdot dp(t) \]

\[ = \psi(\bar{g}(B + v)) - \psi(\bar{g}(B)) = f(B + v) - f(B), \]

where the inequality follows from the monotonicity of \( \psi \), the pointwise antitonicity of the gradient map, the non-negativity of the path, and by linearity of the integral. Hence, \( f \) is submodular. \( \blacksquare \)
We also fairly quickly get a partial corollary where we need not assume that \( \phi \) is monotone non-decreasing.

In the below, let \( b \in \mathbb{R}_+^y \) be a non-negative real vector and for any set \( A \subseteq V \), \( b_A \) is a vector such that \( b_A(v) = b(v) \) if \( v \in A \) and otherwise \( b_A(v) = 0 \) (e.g., when \( b = 1 \) then \( b_A = 1_A \) is the characteristic vector of set \( A \)).

**Corollary 5.12.1.** Let \( \psi : \mathbb{R}^n \to \mathbb{R} \) be any concave function and \( b \in \mathbb{R}_+^y \) be a non-negative real vector.

Then if \( \psi \) has an antitone supergradient, then the set function \( f : 2^V \to \mathbb{R} \) defined as \( f(A) = \psi(b_A) \) for all \( A \subseteq V \) is submodular.

**Proof.** The proof is practically the same as that of Theorem 5.12 except we cannot use the monotonicity of \( \psi \).

In the below, let \( x \) and \( y \) be a non-negative real vector and for any set \( v \in V \), \( b_v \) is a vector such that \( b_v(v) = b(v) \) if \( v \in A \) and otherwise \( b_v(v) = 0 \). Then if \( \phi \) is monotone non-decreasing, \( \int_p \nabla \psi(b_B + z) \cdot dz = \psi(b_B + v) - \psi(b_B) = f(B + v) - f(B) \).

Alternatively, we can set \( k = n \) in Theorem 5.12 and for all \( v \in V \), let \( g_v(A) = b(v)1_{v \in A} \) which is a modular function. Then, the same relative path can be used to move from \( b_A \) to \( b_{A+v} \) as from \( b_B \) to \( b_{B+v} \), so only antitonicity of \( \psi \) is needed in the integral.

Given the above, the following result is not surprising.

**Lemma 5.13.** Let \( \psi : \mathbb{R}^n \to \mathbb{R} \) be a concave function formed by the sum of compositions of a scalar concave function and a linear function, \( i.e., \psi(x) = \sum_i w_i \phi_i((m_i, x)) + \sum m_i \) where \( m_i \in \mathbb{R}_+^y \), \( w_i \geq 0 \) for all \( i \), and \( m_\pm \in \mathbb{R}^n \). Then \( \psi(x) \) has an antitone superdifferential.

**Proof.** From the chain rule, we get that \( \nabla \psi(x) = \sum_i w_i \phi_i'(((m_i, x))m_i^T + m_i^T \) is non-negative, \( w_i \phi_i'(((m_i, x))m_i^T \) is monotone non-increasing in \( x \) (\( m_i^T \) is constant). In the non-differentiable case, \( \phi_i \) being monotone-concave implies that the same is true for any supergradient map. Closure over sums is immediate.

**Corollary 5.13.1.** Any linear function has an antitone superdifferential.

**Lemma 5.14.** Composition of monotone non-decreasing scalar concave and antitone superdifferential concave functions preserves superdifferential antitonicity.

**Proof.** Let \( \phi : \mathbb{R} \to \mathbb{R} \) be a monotone non-decreasing concave function and \( \chi : \mathbb{R}^n \to \mathbb{R} \) be a monotone non-decreasing concave function with an antitone superdifferential, and define \( \psi(x) = \phi(\chi(x)) \).

**Corollary 5.14.1.** The root concave function \( \psi_x \) associated with a DSF has an antitone superdifferential.

**Proof.** The proof follows immediately from the fact that a DSF function (Equation (11)) is a recursive application of composition of monotone concave functions, non-negative sums of monotone concave functions, and the addition of a final linear function associated with \( m_\pm \).

While having an antitone superdifferential is sufficient to yield a submodular function, it is not necessary. Consider the following concave extension of a monotone non-decreasing submodular function [152, 113, 45], \( \psi(x) = \min_{S \subseteq V} \{ f(S) + \sum_{v \in V} x(v)f(v|S) \} \). This function is concave and is tight \( f(A) = \psi(1_A), \forall A \) at the vertices of the unit hypercube, but is not the concave closure of \( f \) [152]. The superdifferential is given by

\[
\partial \psi(x) = \left\{ (f(v_1|S_x), f(v_2|S_x), \ldots, f(v_n|S_x)) : S_x \in \arg\min_{S \subseteq V} \{ f(S) + \sum_{v \in V} x(v)f(v|S) \} \right\} \tag{43}
\]

and when evaluating at \( x = 1_A \) we have \( M_A \triangleq \arg\min_{S \subseteq V} \{ f(S) + \sum_{v \in V} 1_A f(v|S) \} = \{ A \} \cup \{ A' : A' = A - v, \forall v \in A \} \).

To have an antitone supergradient, we need for all \( x \leq y \) and \( g_x \in \partial \psi(x) \), \( g_y \in \partial \psi(y) \), that \( g_x \geq g_y \). Taking \( x = 1_A \) and \( y = 1_{A+v} \) for some \( v \notin A \), we can choose \( A \in M_A \) and \( A' = (A + v - v') \in M_{A+v} \) with \( v' \notin A \). In this case, we can find a monotone submodular function with \( f(v|A) < f(v|A + v - v') \) which violates antitonicity.
In order to explore this further, we consider the case where the function \( \psi \) is twice differentiable. In this case, if \( \psi \) is concave, then an antitone superdifferential means for all \( x \leq y \), we have for all \( i, j \), \( \frac{\partial^2 \psi}{\partial x_i \partial x_j} (x) \geq 0 \). Setting \( y = x + \epsilon 1_{V_i} \), we get for all \( i, j \)

\[
\frac{\partial^2 \psi}{\partial x_i \partial x_j} (x) = \lim_{\epsilon \to 0} \frac{\frac{\partial \psi}{\partial x_i} (x + \epsilon 1_{V_i}) - \frac{\partial \psi}{\partial x_i} (x)}{\epsilon} \leq 0,
\]

which is thus also a sufficient condition for \( f(A) = \psi(1_A) \) being submodular. The condition is stricter than necessary, however. Consider the quadratic \( \psi: \mathbb{R}^2 \to \mathbb{R} \) with \( \psi(x) = x^T \begin{pmatrix} -1 & -2 \\ 1 & 0 \end{pmatrix} x + 41^T x \). Since \( \phi(0, 0) = 0, \phi(0, 1) = 5, \phi(1, 0) = 5, \) and \( \phi(1, 1) = 6, f(A) = \phi(1_A) \) is monotone submodular. Here, we have \( \frac{\partial^2 \psi}{\partial x_i \partial x_j} = -4 \) but \( \frac{\partial^2 \psi}{\partial x_i \partial x_j} = 2 \) for \( i \in \{1, 2\} \). Being submodular does not require the non-positivity of the diagonal elements of the Hessian matrix. In fact, the following weaker sufficient condition for submodularity (an old result, going back more than a hundred years [5, 38, 132, 99, 133, 148, 149]) is well established:

**Theorem 5.15.** Let \( \phi: \mathbb{R}^n \to \mathbb{R} \) be a twice differentiable function. If for all \( i \neq j \) we have \( \frac{\partial^2 \phi}{\partial x_i \partial x_j} \leq 0 \) then the function \( f: 2^V \to \mathbb{R} \) where \( f(A) = \phi(1_A) \) is submodular.

The above result is equivalent to \( \partial \phi(x)/\partial x_j \) being decreasing in \( x_i \) for all \( i \neq j \). This suggests that the antitone superdifferential condition can also be weakened while still ensuring submodularity. Define \( \tilde{d}_i^j \psi(x) = \psi(x + \epsilon 1_{V_i}) - \psi(x) \). Then an antitone superdifferential is the same as, for all \( x \leq y \) having \( \tilde{d}_i^j \psi(x) \geq \tilde{d}_i^j \psi(y) \) for all \( i \) and \( \epsilon > 0 \). This implies that \( \tilde{d}_i^j \tilde{d}_i^j \psi(x) \leq 0 \) for all \( i, j \). The weaker condition asks that \( \tilde{d}_i^j \tilde{d}_i^j \psi(x) \leq 0 \) for all \( i \neq j \), and \( \epsilon > 0 \), and this is the same as

\[
\psi(x + \epsilon 1_{V_i}) + \psi(x + \epsilon 1_{V_j}) \geq \psi(x + \epsilon 1_{V_i} + \epsilon 1_{V_j}) + \psi(x)
\]

which essentially is a restatement of the property of submodularity but on the reals. Note that when \( i = j \), this (and \( \partial^2 \phi(\partial x_i^2) \leq 0 \) in the twice differentiable case) asks for the function to be concave in the direction of each axis, but submodularity, as Theorem 5.15 states, does not require this. Indeed, submodularity is a relationship between distinct variables, not a criterion on any one particular variable.

The weaker condition (Theorem 5.15) is also not necessary for concavity, as the aforementioned quadratic is neither concave nor convex. Concavity requires non-positive definiteness of the Hessian matrix, something that antitone maps do not ensure. A map is any function \( h: \mathbb{R}^V \to \mathbb{R}^V \) and is antitone if for all \( x, y \in \mathbb{R}^V \), \((x - y)^T (h(x) - h(y)) \leq 0 \) for all \( x, y \). Not only does an antitone map alone not ensure concavity (a result established originally in [128, 129]), an antitone map need not be a gradient field (a property that, if true, would make it a conservative field). For an example related to submodular functions, the multilinear extension [119], defined as:

\[
\hat{f}(x) = \sum_{S \subseteq V} f(V) \prod_{i \in S} x_i \prod_{j \in V \setminus S} (1 - x_j)
\]

has the property that \( \hat{f}(1_A) = f(A) \) for all \( A \subseteq V \). It has been used as a extension of a submodular function, surrogate to the true concave envelope, for use in submodular maximization problems [41, 24, 8]. When \( f \) is submodular, it has \( \partial^2 f(x)/\partial x_i \partial x_j \leq 0 \) for all \( i, j \), not only abiding Theorem 5.15 but also for \( i = j \) it has \( \partial^2 \phi/\partial x_i^2 = 0 \) since it is multilinear. Hence, multilinear extension also has an antitone map, but is also neither convex nor concave and hence has neither a subdifferential nor a superdifferential. Indeed, concavity is not at all required for an extension of a submodular function, another well-known example being the Lovász extension of \( f: \mathbb{R}^V \to \mathbb{R} \) of \( x \) which is a convex, has \( f(A) = \hat{f}(1_A) \), is defined as \( \hat{f}(x) = \sum_{i=1}^n x_i \hat{f}(\sigma) \) where \( \sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n) \) is a \( n \)-dependent order ensuring \( x_{\sigma_1} \geq x_{\sigma_2} \cdots \geq x_{\sigma_n} \). \( \hat{f} \) is not twice differentiable but it has a subgradient \( g \in \partial \hat{f}(x) \) where \( g(i) = f(\sigma_i \sigma_1, \sigma_2, \ldots, \sigma_{i-1}) \). Given \( x \leq y \), a decreasing order of \( y \) can be arbitrarily different than for \( x \) implying \( \partial \hat{f}(x) \) is neither antitone nor monotone, so \( \partial^2 \partial^2 \hat{f}(x) \leq 0 \) is not a property of the Lovász extension. Also, any function defined only on the vertices of the unit hypercube has an infinite number of both concave and convex extensions [28]. The approach above shows that antitone superdifferentials involves both concavity and submodular functions. Since Theorem 5.15 does not require concavity, however, this suggests that there may be a way to define submodular functions using generalized line integrals of antitone maps without needing concavity [131].
We also note that Theorem 5.15 is given as a sufficient condition, but not a necessary condition, for submodularity when we consider \( \phi \) as a function used to produce \( f(A) = \phi(1_A) \). Let \( \phi \) be any function satisfying Theorem 5.15 and \( \chi \) be any other function having \( \chi(1_A) = 0 \) for all \( A \subseteq V \). Then \( f(A) = \phi(1_A) + \chi(1_A) \) is submodular while \( \phi(x) + \chi(x) \) need not satisfy the theorem. Theorem 5.15 is typically stated as both necessary and sufficient conditions for submodularity [38, 132, 133, 148, 149], as it is used to define submodularity on those lattices, including the reals (and hence this is sometimes called continuous submodularity), where twice differentiability everywhere is well defined. For example, defining \( \partial_i f(A) = f(A \cup \{ i \}) - f(A \setminus \{ i \}) \) for \( i \in V \), we have that a function \( f : 2^V \rightarrow \mathbb{R} \) is submodular if and only if for \( i \neq j \), \( \partial_i \partial_j f(A) \leq 0 \). This is in contrast to how we use it above, which to define a submodular function only on the unit hypercube vertices starting from a function defined on \( \mathbb{R}^n \).

Getting back to DSFs, since the concave function associated with a DSF has an antitone superdifferential, and since this is sufficient but not necessary for submodularity, this suggests (but does not guarantee, since DSFs evaluate \( \psi \) only at hypercube vertices \( 1_A \)) that the family of DSFs might not comprise all submodular functions. While in Section 6 we show that DSFs generalize SCMMs, and in Section 6.2 we show that increasing the layers in a DSF increases the size of the family, Section 6.3 shows, by giving an example, that not all submodular function can be represented by DSFs.

In closing this section, we state an additional potential advantage of DSFs. Ordinarily the concave closure of a submodular function is computationally hard to evaluate [152] and this is disappointing since such a construct would be useful for relaxation schemes for maximizing submodular functions (and as result surrogates, such as the multilinear extension are used). In the DSF case, however, a particular concave extension is very easy to get, namely \( \psi(x) + (m_+, x) \). This extension perhaps could be useful for maximizing DSFs, possibly constrainedly, using concave maximization followed by appropriate rounding methods.

### 5.3 The Special Matroid Case and Deep Matroid Rank

We discuss in this section the special case of matroids and matroid ranks as they motivate and offer insight to the results later in the paper.

A matroid \( M \) [46] is a set system \( (V, \mathcal{I}) \) where \( \mathcal{I} = \{I_1, I_2, \ldots\} \) is a set of subsets \( I_i \subseteq V \) that are called independent. A matroid has the property that \( 0 \in \mathcal{I} \), that \( \mathcal{I} \) is subclusive (i.e., given \( I \in \mathcal{I} \) and \( I' \in \mathcal{I} \) then \( I' \subseteq I \)) and that all maximally independent sets have the same size (i.e., given \( A, B \in \mathcal{I} \) with \( |A| < |B| \), there exists a \( b \in B \setminus A \) such that \( A + b \in \mathcal{I} \)). The rank of a matroid, a set function \( r : 2^V \rightarrow \mathbb{Z}_+ \) defined as \( r(A) = \max_{I \in \mathcal{I}} |I \cap A| \), is a powerful class of submodular functions. All matroids are defined uniquely by their rank function as \( \mathcal{I} = \{ A : r(A) = |A| \} \) and therefore, we can reason about if two matroids are equivalent or not based on if their ranks are equal, and vice versa. All monotone non-decreasing non-negative integral submodular functions can be exactly represented by grouping and then evaluating grouped ground elements in a matroid [46].

A useful matroid in machine learning applications [94, 9] is the partition matroid, where a partition \( (V_1, V_2, \ldots, V_t) \) of \( V \) is formed, along with a set of capacities \( k_1, k_2, \ldots, k_t \in \mathbb{Z}_+ \). It’s rank function is defined as: \( r(X) = \sum_{i=1}^t \min(|X \cap V_i|, k_i) \) and, therefore, is an SCMM.

A cycle matroid is a different type of matroid based on a graph \( G = (V, E) \) where the rank function \( r(A) \) for \( A \subseteq E \) is defined as the size of the maximum “spanning forest” (i.e., a spanning tree for each connected component) in the edge-induced subgraph \( G_A = (V, A) \). From the perspective of matroids, we can consider classes of submodular functions via their rank. If a given type of matroid cannot represent another kind, their ranks lie in distinct families. To study where DSFs are situated in the space of all submodular functions, it is useful first to study results regarding matroid rank functions.

**Lemma 5.16.** There are partition matroids that are not cycle matroids.

**Proof.** Consider the partition matroid over \(|V| = 4\) elements and consider a partition with one block and a capacity of two, so \( r(X) = \min(|X|, 2) \), so any two elements has rank 2. For this matroid to be a cyclic matroid, we must have a graph with 4 edges where every set of three (out of those 4) must contain a cycle. Let us name the edges \( a, b, c, d \), then \( a, b, c \) contains a cycle and so does \( a, b, d \), while \( a, b \) does not contain a cycle \( \{a, b\} \) has rank 2). The only way this can happen is if either \( c, d \) are parallel edges, or of \( c \) is parallel to one of \( a \) or \( b \), and \( d \) is also parallel to one of \( a \) or \( b \), or if \( c \) and \( d \) are loops. In any of the above

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Lemma 5.17. Laminar matroids strictly generalize partition matroids

Consider a simple laminar family $\mathcal{F} = \{V, F_1, F_{11}, F_{12}, F_2, F_{21}, F_{22}\}$; Middle: the tree structure of the laminar family; Right: a possible corresponding DSF DAG associated with the laminar matroid rank function when $|V| = 14$.

In a laminar matroid, a generalization of a partition matroid, we start with a set $V$ and a family $\mathcal{F} = \{F_1, F_2, \ldots \}$ of subsets $F_i \subseteq V$ that is laminar, namely that for all $i \neq j$ either $F_i \cap F_j = \emptyset$ or $F_i \subseteq F_j$ or $F_j \subseteq F_i$ (i.e., sets in $\mathcal{F}$ are either non-intersecting or comparable). In a laminar matroid, we also have for every $F \in \mathcal{F}$ an associated capacity $k_F \in \mathbb{Z}^+$. A set $I$ is independent if $|I \cap F| \leq k_F$ for all $F \in \mathcal{F}$. A laminar family of sets can be organized in a tree, where there is one root $R \in \mathcal{F}$ in the tree that, w.l.o.g., can be $V$ itself. Then the immediate parents $\text{pa}(F) \subset \mathcal{F}$ of a set $F \in \mathcal{F}$ in the tree are the set of maximal subsets of $F$ in $\mathcal{F}$, i.e., $\text{pa}(F) = \{F' \in \mathcal{F} : F' \subseteq F \text{ and } \not\exists F'' \in \mathcal{F} \text{ s.t. } F' \subseteq F'' \subseteq F\}$. We then define the following for all $F \in \mathcal{F}$:

$$r_F(A) = \min(\sum_{F' \subseteq \text{pa}(F)} r_{F'}(A \cap F') + |A \setminus \bigcup_{F' \subseteq \text{pa}(F)} F'|, k_F).$$

A laminar matroid rank has a recursive definition $r(A) = r_R(A) = r_V(A)$. Hence, if the family $\mathcal{F}$ forms a partition of $V$, we have a partition matroid. More interestingly, when compared to Eqn. (11), we see that a laminar matroid rank function is an instance of a DSF with a tree-structured DAG as shown in Figure 2. Thus, within the family of DSFs lie the truncated matroid rank functions used to show information theoretic hardness for many constrained submodular optimization problems [52], i.e., start with the partition matroid rank $r(A) = \min(|A \cap R|, a) + \min(|A \cap \bar{R}|, |\bar{R}|) = \min(|A \cap R|, a) + |A \cap \bar{R}|$ and then truncate it as follows:

$$f_R(A) = \min\{r(A), b\} = \min\{|A|, a + |A \cap \bar{R}|, b\}$$

with $a < b$. This is a function where $f_R(R) = a$ and $f_R(A) > a$ for $A \neq R$ and $|A| = |R|$ and can be set up to have most size $\geq |R|$ sets $A$ valued at $f_R(A) = b$. Since this function is used to show hardness for many constrained submodular minimization problems, and since DSFs generalize laminar matroid ranks, this portends poorly for algorithms of the kind found in [70, 117] to achieve fast DSF minimization.

Laminar matroids are more general than partition matroids. From the perspective of matroid rank, we have:

**Lemma 5.17.** Laminar matroids strictly generalize partition matroids

**Proof.** Consider a simple laminar family $\mathcal{F} = \{V, B\}$ where $k_V = 2$, $B \subset V$ with $k_B = 1$, and $|B| \geq 2$ and $|V| \geq |B| + 2$ giving rank function

$$r(X) = \min(\min(|X \cap B|, 1) + |X \setminus B|, 2).$$
Suppose we are given any set of subsets \(\{C_i\}\) of \(V\) and corresponding integer capacities \(\{k_i\}\) giving the submodular function:

\[
r_s(X) = \sum_i \min(|X \cap C_i|, k_i).
\]  

and suppose that \(r_s(X) = r(X)\) which means \(r_s(X)\) must be a matroid rank function. Note that \(k_i \geq 1\) otherwise term \(i\) is vacuous. The \(C_i\) must be disjoint, for if not let \(C_i \cap C_j \neq \emptyset, i \neq j\) and pick \(v \in C_i \cap C_j\), which gives \(r_s(v) \geq 2\) implying \(r_s\) is not a matroid rank function. Hence the sets \(C_i\) must be disjoint and \(r_s\) is a partition rank function over \(\cup_i C_i\). Choose two elements \(b_1, b_2 \in B\). If \(b_1 \in C_i\) and \(b_2 \in C_j\) for \(i \neq j\) this gives \(r_s(\{b_1, b_2\}) = 2 \neq r(\{b_1, b_2\}) = 1\). Hence, there is a unique \(i\) such that \(B \subseteq C_i\). Thus, \(k_i = 1\) since if not we would get \(r_s(\{b_1, b_2\}) = 2\). If there exists a \(v \in C_i \setminus B\) then for any \(b \in B\), \(r_s(v, b) = 1 \neq r(v, b)\). Hence, we must have \(C_i = B\). Now take \(v_1, v_2 \notin B\) so that \(r(\{v_1, v_2\}) = r_s(\{v_1, v_2\}) = 2\), but the term of \(r_s\) involving \(B\) does not involve \(v_1, v_2\) so that for \(b \in B\), \(r_s(\{v_1, v_2, b\}) = 3\) which is a contradiction. Hence, a laminar matroid is a strict generalization of a partition matroid. 

Since a laminar matroid generalizes a partition matroid, this augurs well for DSFs generalizing SCMMs (a result we provide in Theorem 6.4). Before considering that, we already are up against some limits of laminar matroids, i.e.: 

**Lemma 5.18.** Laminar matroid cannot represent all cycle matroids. 

**Proof.** Consider the cycle matroid over edges on \(K_4\), hence \(M = (V, \mathcal{I})\) with \(|V| = 6\), \(V\) being the set of edges, where \(r(X) = |X|\) for \(|X| \leq 2\), \(r(X) = 2\) when \(X\) is any 3-cycle, \(r(X) = 3\) for any acyclic \(X\) with \(|X| > 3\). Consider the form of the laminar matroid in Eqn. (47) and suppose \(r_{\mathcal{V}}(X) = r(X)\) for all \(X\). W.l.o.g., we may assume \(k_{\mathcal{V}} = 3\). Suppose \(\exists e \in V \setminus \cup_{F \in \text{pa}(V)} F\). Then consider any 3-cycle \(C\) involving \(e\), and \(r_{\mathcal{V}}(C - e) = 2\) but since no element of \(\text{pa}(V)\) contains \(e\), there is no truncation, giving \(r_{\mathcal{V}}(C) = 3\), a contradiction. Hence, \(V = \cup_{F \in \text{pa}(V)} F\). Given a 3-cycle \(C = \{a, b, c\}\), suppose there exists an \(F \in \text{pa}(V)\) with \(a \in F\) and \(b \notin F\) and \(c \notin F\). Since we must have \(r_{\mathcal{V}}(\{b, c\}) = 2\) and \(r_{\mathcal{V}}(\{a\}) = 1\), this implies \(r_{\mathcal{V}}(\{a, b, c\}) = 3\), also a contradiction. Hence, any three cycle must be in one element of \(\text{pa}(V)\), and by transitive closure over the four intersecting three-cycles, all elements of \(V\) must be in only one member of \(\text{pa}(V)\). This implies that \(|\text{pa}(V)| = 1\) and the only way to represent the 3-cycles is within that one term, \(r_F(X)\). This process then is applied recursively until we are left with the base case, where the entire recursion boils down to the form \(r_{\mathcal{V}}(X) = \min(r_F(X), 3) = \min(\min(|X|, k_F), 3) = \min(|X|, \min(k_F, 3))\). This clearly cannot represent the cycle matroid rank function for any value of \(k_F \in \mathbb{Z}_+\). 

The proof technique is reminiscent of the back propagation method used to train DNNs and hence we call it “backprop proof” — it recursively backpropagates required properties from the root though each layer (in a DSF sense) of a laminar matroid rank function until it boils down to a partition matroid rank function, where the base case is clear. The proof is elucidating since it motivates the proof of Theorem 6.4 showing that DSFs extend SCMMs. We also have the immediate corollary.

**Corollary 5.18.1.** Partition matroids cannot represent all cycle matroids.

### 5.4 Surplus and Absolute Redundancy

In this section, we introduce and study the notion of the surplus of a set as measured by a submodular function. The surplus is a useful concept and will be used extensively to show, in Section 6, various properties of the DSF family.

**Definition 5.19 (Surplus and Absolute Redundancy).** For a function \(f : 2^V \to \mathbb{R}\), we define \(\mathcal{J}_f(A)\) as the surplus (or absolute redundancy) of a set \(A \subseteq V\) by \(f\) as follows:

\[
\mathcal{J}_f(A) = \sum_{a \in A} f(a) - f(A)
\]  

(51)
We call \( \mathcal{S}_f(A) \) the surplus of \( A \) by \( f \). We use the term “surplus” under an interpretation where \( A \) is a set of agents that can perform their action either independently of each other, or may perform their actions jointly and cooperatively [149]. If an agent \( a \in A \) performs the action independently, the cost is \( f(a) \) with an overall cost of \( \sum_{a \in A} f(a) \), while if the agents \( A \) perform the action cooperatively, the overall cost is \( f(A) \). The difference \( \mathcal{S}_g(A) = \sum_{a \in A} f(a) - f(A) \) is the surplus obtained by performing the actions \( A \) cooperatively rather than individually. When \( g \) is submodular, surplus is never negative. Hence, performing the actions jointly leads overall to profit.\(^3\)

The idea of surplus has occurred before in the field of information theory but under a different name — in this case, \( f(A) = H(X_A) \) is the entropy function of a set of random variables indexed by the set \( A \). The quantity \( \mathcal{S}_f(A) = \sum_{a \in A} H(X_a) - H(X_A) \) is the average bit-length penalty between optimally coding the random variables in \( A \) separately (as if they were independent) vs. optimally coding them jointly. This can, thus, be called the absolute redundancy of the set \( A \). For the entropy function, this idea was first defined in [102].\(^4\) Absolute redundancy is also called “total correlation” [154] and also the “multi-information” function [143]. Our notion of surplus is not the same as [118] where they define a quantity called “deficiency” the negative of which may be considered a kind of surplus. Since there may neither be a statistical, information theoretic, nor economic interpretation, we actually prefer the terms “total interaction” or “combinatorial interaction.” In the below, if only for the sake of brevity, we utilize the term “surplus,” but stress that it applies to any submodular function whatever its interpretation. We say that the function \( g \) “gives surplus” to a set \( A \) whenever \( \mathcal{S}_g(A) > 0 \) and otherwise \( A \) has “no surplus.”

In the below, we explore a number of properties and introduce a number of variants of surplus, all of which are useful later in the paper.

**Lemma 5.20 (Linearity of Surplus).** Let \( f_1, f_2 \) be two functions and \( \alpha_1, \alpha_2 \in \mathbb{R}_+ \). Then for any \( A \subseteq V \)

\[
\mathcal{S}_{\alpha_1 f_1 + \alpha_2 f_2}(A) = \alpha_1 \mathcal{S}_{f_1}(A) + \alpha_2 \mathcal{S}_{f_2}(A)
\] (52)

**Lemma 5.21 (Surplus is Immune to Modularity).** Modular functions do not change surplus, i.e., when \( m : V \rightarrow \mathbb{R} \) is a normalized modular function and \( f \) is any set function:

\[
\mathcal{S}_{f+m}(A) = \mathcal{S}_f(A)
\] (53)

That modular functions do not influence surplus is useful to be able to ignore the final modular function \( m_{\pm} \) in a DSF when studying its properties.

**Lemma 5.22 (Non-negativity of Surplus).** When \( f \) is normalized (\( f(\emptyset) = 0 \)) and submodular, then for all \( A \subseteq V, \mathcal{S}_f(A) \geq 0 \).

**Proof.** For any \( A \subseteq V \), with \( A = \{a_1, a_2, \ldots, a_k\} \),

\[
f(A) = \sum_{i=1}^k f(a_i|a_1, a_2, \ldots, a_{i-1}) \leq \sum_{i=1}^k f(a_i)
\] (54)

Thus, with a submodular function in such a context, therefore, there can never be any deficit (negative surplus) and it is always beneficial to act cooperatively. How fairly to redistribute surplus back to the individual agents is called the “surplus sharing problem” and is studied in [149].

**Lemma 5.23 (Mixtures Preserve Surplus).** Let \( f_1, f_2, \ldots \) be a set of submodular functions and \( \alpha_1, \alpha_2, \ldots \) be a set of positive real-valued weights, and define \( f = \sum \alpha_i f_i \) as their conic combination. Then we have \( \mathcal{S}_f(A) > 0 \) if and only if \( \exists i \) with \( \mathcal{S}_{f_i}(A) > 0 \).

\(^3\)In [149], surplus is defined as \( f(A) - \sum_{a \in A} f(a) \) where \( f \) is a supermodular function, but the same idea still applies.

\(^4\)Incidentally, in 1954, [102] was also the first, to the authors knowledge, to provide inequalities on the entropy function that are identical to the submodularity condition.

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Proof. This follows when one considers that \( \forall i, \mathcal{I}_f(A) \geq 0 \) for all \( A \), that \( \forall i, \alpha_i > 0 \), and that \( \mathcal{I}_f(A) = \sum_i \alpha_i \mathcal{I}_f(A) \).

The next theorem is particularly important for showing certain properties of DSFs, in particular, Corollary 6.23.1.

**Theorem 5.24 (Concave Composition Preserves Surplus).** Let \( h : 2^V \to \mathbb{R} \) be a polymatroid function and \( \phi : \mathbb{R} \to \mathbb{R} \) be a normalized monotone non-decreasing concave function that is not identically zero. Define \( g : 2^V \to \mathbb{R} \) as \( g(A) = \phi(h(A)) \). Then \( \mathcal{I}_f(h(A)) > 0 \) implies \( \mathcal{I}_g(A) > 0 \).

Proof. Since \( g(\cdot) \) is polymatroidal (by Theorem 5.4), \( \mathcal{I}_g(A) \geq 0 \) for all \( A \). Order \( A \) arbitrarily as \( A = \{a_1, a_2, \ldots, a_k\} \) with \( k = |A| \). Then since \( \sum_{i=1}^k h(a_i) > h(A) \),

\[
\sum_{i=1}^k \phi(h(a_i)) \geq \phi(\sum_{i=1}^k h(a_i)) \geq \phi(h(A)),
\]

where (a) follows from Theorem 5.7 and (b) follows from the monotonicity of \( \phi \). If \( \sum_{i=1}^k h(a_i) \) is still in the linear part of \( \phi(\cdot) \) then (b) is strict, while if \( \sum_{i=1}^k h(a_i) \) is greater than the linear part of \( \phi(\cdot) \) then, from the second part of Theorem 5.7, (a) is strict. In either case, \( \mathcal{I}_g(A) > 0 \).

**Proposition 5.25 (Concave Composition Increases Surplus).** Let \( h : 2^V \to \mathbb{R} \) be a polymatroid function with \( h(v) = 1 \) for all \( v \in V \), and \( \phi : \mathbb{R} \to \mathbb{R} \) be a normalized monotone non-decreasing concave function that is not identically zero and where \( \phi(1) = 1 \). Define \( g : 2^V \to \mathbb{R} \) as \( g(A) = \phi(h(A)) \). Then for any \( A \), \( \mathcal{I}_g(A) \geq \mathcal{I}_h(A) \).

**Definition 5.26 (Grouped Surplus).** We define a form of grouped surplus as follows. Given a set of \( m \) disjoint sets \( A_1, A_2, \ldots, A_m \subseteq V \), we define:

\[
I_f^{(m)}(A_1; A_2; \ldots; A_m) \triangleq \sum_{i=1}^m f(A_i) - f(\bigcup_{i=1}^m A_i)
\]

When \( f(A) = H(X_A) \) is the entropy function, then the pairwise surplus \( I_f^{(2)}(A; B) \) is the well-known mutual information [27] between random variable sets \( X_A \) and \( X_B \). The grouped surplus can be defined in terms of standard surplus via \( I_f^{(m)}(A_1; A_2; \ldots; A_m) = \mathcal{I}_f(\{A_1\}, \{A_2\}, \ldots, \{A_m\}) \) where we treat each of the sets \( \{A_i\} \) as a singleton element groups in the standard surplus. Thus, for any \( m \), we have \( I_f^{(m)}(A_1; A_2; \ldots; A_m) \geq 0 \) for any normalized submodular function \( f \). We also have the following:

**Proposition 5.27.** Given a submodular function \( f \) and a set \( A \subseteq V \), if \( \mathcal{I}_f(A) = 0 \) then \( I_f^{(m)}(A_1; A_2; \ldots; A_m) = 0 \) for any \( m \) and proper \( m \)-partition \( A_1, A_2, \ldots, A_m \subseteq A \) of \( A \). Moreover, we have:

\[
\mathcal{I}_f(\bigcup_{i=1}^m A_i) > I_f^{(m)}(A_1; A_2; \ldots; A_m)
\]

For example, if \( I_f^{(2)}(A; B) = 0 \) then \( \mathcal{I}_f(A \cup B) = 0 \). The converse is not true in general, i.e., we can have \( I_f^{(2)}(A; B) = 0 \) while still having \( \mathcal{I}_f(B) > 0 \). Of particular interest in this paper will be pairwise surplus of the form \( I_f^{(2)}(e'; C) \) where \( C \) is a three-cycle of a graphic matroid, and \( e' \notin C \). When it is clear from the context, we will drop the superscript \( m \) and state \( I_f(A_1; A_2; \ldots; A_m) \triangleq I_f^{(m)}(A_1; A_2; \ldots; A_m) \) for any \( m \). Considering Proposition 5.27 and Definition 5.26, we immediately obtain the following:

**Proposition 5.28 (Concave Composition Preserves Grouped Surplus).** Let \( h : 2^V \to \mathbb{R} \) be a polymatroid function and \( \phi : \mathbb{R} \to \mathbb{R} \) be a normalized monotone non-decreasing concave function that is not identically zero. Define \( g : 2^V \to \mathbb{R} \) as \( g(A) = \phi(h(A)) \). Then for any \( m \) and any set of \( m \) disjoint sets \( A_1, A_2, \ldots, A_m \), we have \( I_h^{(m)}(A_1; A_2; \ldots; A_m) > 0 \) implies \( I_g^{(m)}(A_1; A_2; \ldots; A_m) > 0 \).
**Definition 5.29** (Modular at B). We say a function $h : 2^V \to \mathbb{R}$ is modular at $B \subseteq V$ if $h(B) = \sum_{b \in B} h(b)$.

When $h$ is modular at $B$, it does not necessarily mean that it is modular at some $A \subseteq B$. However, we do have the following:

**Lemma 5.30.** If $h : 2^V \to \mathbb{R}$ is a submodular function. Then $h$ is modular at all $A \subseteq B$ if and only if $\mathcal{J}_h(B) = 0$.

**Proof.** If $h$ is modular for all $A \subseteq B$, then $h(A) = \sum_{a \in A} h(a)$, and $\mathcal{J}_h(B) = 0$. Conversely, suppose $h$ is submodular and $\mathcal{J}_h(B) = 0$ and let $A \subseteq B$ be given. Then

$$h(B) = \sum_{b \in B} h(b) \geq h(A) + \sum_{b \in B \setminus A} h(b) \geq h(B)$$

(58)

Hence, all inequalities are equalities. Subtracting $\sum_{b \in B \setminus A} h(b)$ from both sides of the first inequality gives the result.

**Lemma 5.31** (Forced Separation). Let $h : 2^V \to \mathbb{R}$ be a polymatroid function and $A, B, C$ be disjoint subsets where $I_h(A; B) = I_h(B; C) = I_h(C; A) = 0$. Then if $h(A) = 0$ then $I_h(A; B; C) = 0$.

**Proof.** Consider the following:

$$h(A) + h(B) + h(C) = h(B) + h(C) = h(B \cup C) \leq h(A \cup B \cup C)$$

(59)

$$\leq h(A) + h(B \cup C) = h(B \cup C),$$

(60)

where the first equality is because $h(A) = 0$, the next is since $I_h(B; C) = 0$, the next (an inequality) is due to monotonicity, the subsequent inequality is due to submodularity, and the final one is since $h(A) = 0$. Hence, all inequalities are equalities, and $I_h(A; B; C) = 0$.

As an example, if $A = \{a\}$, $B = \{b\}$, $C = \{c\}$, then the consequence of the lemma is that $h$ would be modular at the set $\{a, b, c\}$.

The next lemma shows how we can hold the surplus of a set accountable either to the concave function of a concave composition function or to somewhere else internal in the polymatroid function.

**Lemma 5.32** (When Concave Composition Is Linear). Let $h : 2^V \to \mathbb{R}$ be a polymatroid function and $\phi : \mathbb{R} \to \mathbb{R}$ be a normalized monotone non-decreasing concave function that is not identically zero. Define $g : 2^V \to \mathbb{R}$ as $g(X) = \phi(h(X))$ for any $X \subseteq V$. Given two disjoint sets $A, B \subseteq V$ where $g(A) > 0$, $g(B) > 0$, and $I_g(A; B) = 0$, then any surplus $\mathcal{J}_g(A) > 0$ given to $A$ is not due to any non-linearity in $\phi(\cdot)$ but rather is due entirely to $h(\cdot)$. Moreover, $g(X) = \gamma h(X)$ for all $X \subseteq A \cup B$ for some $\gamma > 0$.

**Proof.** By Theorem 5.24, $I_g(A; B) = 0$ implies that $I_h(A; B) = 0$. Then we have

$$\phi(h(A)) + \phi(h(B)) = \phi(h(A \cup B)) = \phi(h(A) + h(B)).$$

(61)

Also, $g(A) > 0 \Rightarrow h(A) > 0$ and $g(B) > 0 \Rightarrow h(B) > 0$. Hence, by Theorem 5.6, $\phi(\cdot)$ is linear in the range $[0, h(A) + h(B)]$.

### 6 The Family of Deep Submodular Functions

We have seen that SCMMs generalize partition matroid rank functions and DSFs generalize laminar matroid rank functions. We might expect, from the above results, that DSFs might strictly generalize SCMMs — this is not immediately obvious since SCMMs are significantly more capable than partition matroid rank functions because: (1) the concave functions need not be simple truncations at integers, (2) each term can have its own non-negative modular function, (3) there is no requirement to partition the ground elements over terms in an SCMM, and (4) we are allowed with SCMMs to add an additional arbitrary modular function. We also have already seen Theorem 5.8 showing that SCMMs are a larger class of submodular functions than just one concave over modular function and, in Lemma 5.10, that they generalize weighted cardinality.
truncations. SCMMs seem therefore to be quite dexterous. The next several sections show, however, that DSFs strictly generalize SCMMs.

More specifically, we formally place DSFs within the context of general submodular functions. We show in Section 6.1 that DSFs strictly generalize SCMMs while preserving many of their attractive attributes (i.e., featurization, multi-modal, and amenability to learning, streaming, and parallel optimization). Then in Section 6.2, we show that the family of DSFs strictly grow with the number of layers uses. In Section 6.3, however, we show that the family of DSFs still do not comprise all submodular functions. We summarize the results of this section in Figure 4, and that includes familial relationships amongst other classes of submodular functions (e.g., various matroid rank functions mentioned in Section 5.3).

6.1 DSFs generalize SCMMs

It is clear that DSFs contain at least the class of SCMMs since any one-layer DSF is an SCMM. We next show that $\text{SCMM} \subseteq \text{DSF}$ holds, or that DSFs strictly generalize SCMMs, thus providing justification for using DSFs over SCMMs and, moreover, generalizing Lemma 5.17 to the non matroid case. The first DSF we choose is a laminar matroid, so SCMMs are unable to represent laminar matroid rank functions even given their additional flexibility over partition matroid rank functions. Since DSFs generalize laminar matroid rank functions, the result follows.

It is not immediately apparent that DSFs generalize SCMMs as the following example demonstrates. Consider the DSF $f : 2^V \to \mathbb{R}$ where $V = \{a, b, c, d, e, f\}$:

$$
f(A) = \min \left( \min(|A \cap \{a, b, c\}|, 1) + \min(|A \cap \{d, e, f\}|, 1), 1.5 \right)
$$

(62)

The reader is encouraged to ponder, for a moment, how one might represent this DSF as an SCMM. Indeed, this is one case where it is possible, as seen by the following SCMM $g : 2^V \to \mathbb{R}$

$$
g(A) = \phi(|A \cap \{a, b, c\}|) + \phi(|A \cap \{d, e, f\}|) + \min(|A|, 0.5) - 0.5|A|
$$

(63)

where $\phi : \mathbb{R} \to \mathbb{R}$ is concave, with $\phi(\alpha) = \min(\alpha, 0.5 + 0.5\alpha)$. It can be verified that $g(A) = f(A)$ for all $A \subseteq V$. In fact, an even simpler SCMM does not use a modular function at all and puts $g(A) = \frac{1}{2} (\min(|A \cap \{a, b, c\}|, 1) + \min(|A \cap \{d, e, f\}|, 1) + \min(|A|, 1))$. From this example, one might naturally surmise that the DSFs unable to be represented by SCMMs are obscure, contrived, and complicated. In the next two sections, however, we show two fairly simple DSFs and show that no SCMM can represent them. Then in Section 6.1.3, we provide more general conditions describing when 2-layer DSF do or do not generalize SCMMs.
6.1.1 The Laminar Matroid Rank Case

Our first example DSF we choose is a simple laminar matroid on six elements. We show that SCMMs cannot express this laminar rank function and since DSFs generalize laminar matroid ranks, the result follows. Consider the following function \( f : 2^V \rightarrow \mathbb{R} \) where \( V = \{a, b, c, d, e, f\} \):

\[
f(A) = \min \left( \min(|A \cap \{a, b, c\}|, 2) + \min(|A \cap \{d, e, f\}|, 2) + 3 \right)
\]

(64)

The function is a laminar matroid rank function with \( \mathcal{F} = \{V, \{a, b, c\}, \{d, e, f\}\} \) and limits \( k_V = 3, k_{\{a,b,c\}} = 2, k_{\{d,e,f\}} = 2 \).

In the following results, we assume that \( g : 2^V \rightarrow \mathbb{R} \) is an SCMM of the form \( g(A) = \sum_{i \in \mathcal{M}} g_i(A) + m_\pm(A) \) where \( g_i(A) = \phi_i(m_i(A)) \) is a normalized monotone non-decreasing concave function composed with a non-negative modular function, \( m_\pm(A) \) is an arbitrary normalized modular function, and \( \mathcal{M} \) is an index set. Since \( f \) itself is normalized, then we must also have \( g(0) = 0 \) as well. Also define \( B_1 = \{a, b, c\} \) and \( B_2 = \{d, e, f\} \).

**Lemma 6.1.** Suppose \( f(A) = g(A) \) for all \( A \). Then there does not exist an \( i \in \mathcal{M} \) where \( g_i \) offers surplus both to \( B_1 \) and \( B_2 \) (i.e., there exists no \( i \) such that \( \mathcal{S}_{g_i}(B_1) > 0 \) and \( \mathcal{S}_{g_i}(B_2) > 0 \)).

**Proof.** Suppose to the contrary that there exists such an \( i \). Then both \( m_i(B_1) \) and \( m_i(B_2) \) must both be past the last linear point of \( \phi_i \), say \( \alpha_i \). We have that

\[
m_i(B_1) + m_i(B_2) = m_i(\{a, b, c\} \cup \{d, e, f\}) = m_i(\{a, b, d\} \cup \{c, e, f\})
\]

(65)

\[
= m_i(\{a, b, d\}) + m_i(\{c, e, f\})
\]

(66)

Since \( m_i(B_1) > \alpha_i \) and \( m_i(B_2) > \alpha_i \) we must have at least one of \( m_i(\{a, b, d\}) > \alpha_i \) or \( m_i(\{c, e, f\}) > \alpha_i \), w.l.o.g., say \( \{a, b, d\} \). This implies that \( \mathcal{S}_{g_i}(\{a, b, d\}) > 0 \) giving \( g \) an unrecoverable surplus which is a contradiction since \( \mathcal{S}_f(\{a, b, d\}) = 0 \).

The next result is our first instance of a DSF that cannot be represented by an SCMM.

**Lemma 6.2.** No SCMM can represent the DSF in Equation (64).

**Proof.** For clarity, we offer the proof as a series of numbered statement groups.

1. Lemma 6.1 means that we can write \( g \) as follows:

\[
g(A) = \sum_{i \in \mathcal{M}_1} g_i(A) + \sum_{i \in \mathcal{M}_2} g_i(A) + \sum_{i \in \mathcal{M}_0} g_i(A)
\]

(67)

where \( \mathcal{M}_0, \mathcal{M}_1, \mathcal{M}_2 \) is a partition of \( \mathcal{M} \), and where for all \( i \in \mathcal{M}_1, g_i \) gives surplus to \( B_1 \) but not to \( B_2 \), for all \( i \in \mathcal{M}_2, g_i \) gives surplus to \( B_2 \) but not to \( B_1 \), and for all \( i \in \mathcal{M}_0, g_i \) gives surplus neither to \( B_1 \) nor \( B_2 \). Hence, for all \( i \in \mathcal{M}_1 \) and \( v \in B_1 \) we have \( g_i(v) > 0 \), and for all \( i \in \mathcal{M}_2 \) and \( v \in B_2 \) we have \( g_i(v) > 0 \) by Lemma 5.31. Furthermore, since \( B_1 \) and \( B_2 \) are the only sets of size three that are given a surplus, then for all \( i \in \mathcal{M}_0, \mathcal{S}_{g_i}(A) = 0 \) for all \( A \) with \( |A| \leq 3 \).

2. We also need to have zero pairwise surplus such as:

\[
I_g(e; \{a, b, c\}) = I_f(e; \{a, b, c\}) = 0
\]

(68)

This implies that for \( i \in \mathcal{M}, I_{g_i}(e; \{a, b, c\}) = 0 \). Since we know that \( m_i(B_1) \) is past the non-linear part of \( \phi_i \) for \( i \in \mathcal{M}_1 \) and \( m_i(B_2) \) is past the non-linear part of \( \phi_i \) for \( i \in \mathcal{M}_2 \), the only way to achieve this (and corresponding values such as \( I_g(b; \{d, e, f\}) = 0 \)) is if both: (1) for \( i \in \mathcal{M}_1, g_i(v) = 0 \) when \( v \in B_2 \); and (2) for \( i \in \mathcal{M}_2, g_i(v) = 0 \) when \( v \in B_1 \).

In other words, \( g_i \) with \( i \in \mathcal{M}_1 \) not only offers no surplus for \( B_2 \) but also give zero valuation for any \( v \in B_2 \) (and vice versa).
3. Consider the following set of size-four sets \( A = \{ A \subseteq V : |A \cap B_1| = |A \cap B_2| = 2 \} \). Note that \(|A| = 9\). For any \( A \in A \), we have
\[
\mathcal{S}_f(A) = \mathcal{S}_g(A) = \sum_{i \in M} \mathcal{S}_{g_i}(A) = 1. \tag{69}
\]
For \( i \in M_1 \cup M_2 \), we have \( \mathcal{S}_{g_i}(A) = 0 \) since two elements of \( A \) are given zero value to every such \( g_i \).

Hence, the only terms that can achieve Equation (69) are those \( i \) within \( M_0 \) having \( \mathcal{S}_{g_i}(A) > 0 \), where \( m_i(A) > \alpha_i \), and where \( \alpha_i \) is the last linear part of \( \phi_i \). Also, to ensure no unrecoverable surplus occurs, we must have that \( m_i(C) \leq \alpha_i \) for any \( C \) having the following properties: (1) any size-three set; (2) any size-four set \( C \) with \(|C \cap B_1| = 3 \) and \(|C \cap B_2| = 1 \) (because \( \mathcal{S}_{g_i}(C \cap B_1) = 0 \) and \( I_{g_i}(C \cap B_1; C \cap B_1) = 0 \)); and (3) any size-four set \( C \) with \(|C \cap B_1| = 1 \) and \(|C \cap B_2| = 3 \). For example, with \( A = \{a, b, d, e\} \) and \( C = \{a, b, c, d\} \), we have that
\[
m_i(a, b, c, d) \leq \alpha_i < m_i(a, b, d, e) = m_i(A) \tag{70}
\]
implying that \( m_i(c) < m_i(e) \).

For any \( A \in A \), define \( A_2(A) = \{ A' \in A : |A' \triangle A| = 2 \} \) and \( A_4(A) = \{ A' \in A : |A' \triangle A| = 4 \} \). Then \(|A_2(A)| = 4\), \(|A_4(A)| = 4\), and \( A = \{A\} \cup A_2(A) \cup A_4(A) \). Suppose \( m_i(A') > \alpha_i \) where \( A' \in A_4(A) \). For example, with \( A = \{a, b, d, e\} \) as above, and \( A' = \{b, c, d, f\} \in A_4(A) \), this implies that \( m_i(d, e, f, b) \leq \alpha_i < m_i(b, c, d, f) \) implying that \( m_i(e) < m_i(c) \), a contradiction with the above. Hence, we must have \( m_i(A') \leq \alpha_i \).

More generally, \( g_i \) offering surplus to more than one member of \( A_4(A) \) leads to a contradiction. Also, if \( A' \in A_4(A) \), then \( \exists A'' \in A_4(A') \) with \( A'' \not= A \) and \( A'' \in A_4(A) \). For example, with \( A \) and \( A' \) given as above, \( A'' = \{a, c, e, f\} \). No more than one of this trio \( \{A, A', A''\} \) can be offered surplus by the same \( g_i \) for \( i \in M_0 \). This means that we may partition the indices \( M_0 = \{M_0^{(0)}, M_0^{(1)}, M_0^{(2)}, M_0^{(3)}\} \) so that \( i \in M_0^{(1)} \) may give surplus to \( A \), but neither \( A' \) nor \( A'' \), \( i \in M_0^{(2)} \) may give surplus to \( A' \) but neither \( A \) nor \( A'' \), \( i \in M_0^{(3)} \) may give surplus to \( A'' \) but neither \( A \) nor \( A' \), and \( i \in M_0^{(0)} \) gives no surplus any of the trio.

We must then have
\[
3 = \mathcal{S}_f(V) = \sum_{j \in \{0, 1, 2\}} \sum_{i \in M_j} \mathcal{S}_{g_i}(V) \tag{71}
\]
\[
\geq \sum_{i \in M_1} \mathcal{S}_{g_i}(B_1) + \sum_{i \in M_2} \mathcal{S}_{g_i}(B_2) + \sum_{i \in M_0} \mathcal{S}_{g_i}(V) \tag{72}
\]
\[= 1 + 1 + \sum_{i \in M_0^{(1)}} \mathcal{S}_{g_i}(V) + \sum_{i \in M_0^{(2)}} \mathcal{S}_{g_i}(V) + \sum_{i \in M_0^{(3)}} \mathcal{S}_{g_i}(V) \tag{73}
\]
\[
\geq 2 + \sum_{i \in M_0^{(1)}} \mathcal{S}_{g_i}(A) + \sum_{i \in M_0^{(2)}} \mathcal{S}_{g_i}(A') + \sum_{i \in M_0^{(3)}} \mathcal{S}_{g_i}(A'') \tag{74}
\]
\[= 2 + 1 + 1 + 1 = 5 \tag{75}
\]
which is a contradiction.

\[\square\]

### 6.1.2 A Non-matroid Case

Lest one thinks it is only the matroids that give difficulty to SCMMs, consider the function \( f : 2^V \rightarrow \mathbb{R} \) where again \( V = \{a, b, c, d, e, f\} \).

\[
f(A) = \min \left( \min(|A \cap \{a, b, c, d\}|, 3) + \min(|A \cap \{c, d, e, f\}|, 3), 5 \right) \tag{76}
\]
Here, there is an overlap between the two sets \( B_1 = \{a, b, c, d\} \) and \( B_2 = \{c, d, e, f\} \). This is not a matroid rank since, for example, \( f(c) = 2 \). Also, minimal sets of maximum value are not all the same size, e.g., \( f(\{a, c, d\}) = 5 \) while \( f(\{a, b, c, e\}) = 5 \).

**Lemma 6.3.** No SCMM can represent the DSF in Equation 76.

**Proof.** For clarity, we offer the proof as a series of numbered statement groups.

1. Assume that for all \( A \subseteq V \), \( f(A) = g(A) = \sum_{i \in \mathcal{M}} g_i(A) \) for some index set \( \mathcal{M} \).

2. Assume \( \exists i \in \mathcal{M} \) that offers surplus both to \( B_1 \) and \( B_2 \). Let \( \alpha_i \) be the last linear point in \( \phi_i \). Then we must have \( m_i(B_1) > \alpha_i \) and \( m_i(B_2) > \alpha_i \), leading to

\[
m_i(B_1) + m_i(B_2) = m_i(B_1 \cap B_2) + m_i(B_1 \triangle B_2)
\]

where \( B_1 \triangle B_2 = (B_1 \setminus B_2) \cup (B_2 \setminus B_1) \) is the symmetric difference between \( B_1 \) and \( B_2 \). Hence we must have at least one of \( m_i(B_1 \cap B_2) > \alpha_i \) or \( m_i(B_1 \triangle B_2) > \alpha_i \). Either case, however, would cause an unrecoverable surplus for sets (either \( B_1 \cap B_2 \) or \( B_1 \triangle B_2 \)) neither of which should be in surplus.

3. We may partition the index set \( \mathcal{M} \) in to \( \mathcal{M}_0, \mathcal{M}_1, \mathcal{M}_2 \) where \( \mathcal{M}_1 \) does not give a surplus to \( B_2 \), \( \mathcal{M}_2 \) does not give a surplus to \( B_1 \), and \( \mathcal{M}_0 \) gives neither to \( B_1 \) nor to \( B_2 \).

4. This leads to too much surplus, i.e.,

\[
1 = \mathcal{I}_f(V) = \sum_{i \in \mathcal{M}} \mathcal{I}_{g_i}(V) = \sum_{i \in \mathcal{M}_0} \mathcal{I}_{g_i}(V) + \sum_{i \in \mathcal{M}_1} \mathcal{I}_{g_i}(V) + \sum_{i \in \mathcal{M}_2} \mathcal{I}_{g_i}(V) \geq \sum_{i \in \mathcal{M}_1} \mathcal{I}_{g_i}(B_1) + \sum_{i \in \mathcal{M}_2} \mathcal{I}_{g_i}(B_2) = 2
\]

a contradiction.

\[\blacksquare\]

**Exercise 6.1.** It is left to the reader to show that the following function can not be represented as an SCMM:

\[
f(A) = \min\left(\sum_{i=1}^{4} \min(|A \cap B_i|, 3), 7\right)
\]

where \( V = \{a, b, c, d, e, f, g, h\} \) and where \( B_1 = \{a, b, c, d\}, B_2 = \{c, d, e, f\}, B_3 = \{e, f, g, h\}, \) and \( B_4 = \{g, h, a, b\} \).

It is also possible to construct a truncated matroid rank function of the kind described in Equation (88) that cannot be represented by an SCMM.

Summarizing the results from the above sections, we have the following.

**Theorem 6.4.** The DSF family is strictly larger than that of SCMMs.

A consequence of this theorem is that in order most generally allow interaction amongst a hierarchy of concepts, as intuitively argued in Section 4, it not sufficient to use solely SCMMs.

### 6.1.3 More General Conditions on Two-Layer Functions

In this section, we revisit again the form of DSF in Equation (64) where we saw there is no corresponding SCMM. Let us slightly generalize Equation (64) in the following.

\[
g(A) = \phi(\min(|A \cap \{a, b, c\}|, 2) + \min(|A \cap \{d, e, f\}|, 2))
\]

where \( \phi \) is normalized monotonically non-decreasing concave function. Lemma 6.2 does not require that for all \( \phi \), the corresponding DSF has no SCMM representation. Indeed, for certain functions \( \phi \) it is possible. While we do not, in this paper, give a complete characterization of those DSFs that can or cannot be represented by SCMMs, we do offer the following theorem.

\[28\]
Theorem 6.5. The function $g(A)$ in Equation 81 is an SCMM if and only if $-\phi(1) + 3.5\phi(2) - 4\phi(3) + 1.5\phi(4) \geq 0$ and $2\phi(1) + \phi(2) - 4\phi(3) + 2\phi(4) \geq 0$.

The proof of the “if” part of this theorem follows by considering the following expression which is clearly an SCMM as long as all of the coefficient are non-negative. The “if” part of the proof is fairly easy — we may simply write $g(A)$ as the form of SCMMs as follows:

$$
g(A) = \left[2\phi(1) + \phi(2) - 4\phi(3) + 2\phi(4)\right] \min(|A \cap \{a, b, c, d, e, f\}|, 1) \tag{82}
+ [-\phi(1) + 3.5\phi(2) - 4\phi(3) + 1.5\phi(4)] \min(|A \cap \{a, b, c, d, e, f\}|, 2) \tag{83}
+ [-\phi(2) + 2\phi(3) - \phi(4)] \left[\min(|A \cap \{a, b, c\}|, 1) + \min(|A \cap \{d, e, f\}|, 1)\right] \tag{84}
+ [\phi(3) + \phi(4)] \left[\min(|A \cap \{a, b, c\}|, 2) + \min(|A \cap \{d, e, f\}|, 2)\right] \tag{85}
+ [-\phi(2) + 2\phi(3) - \phi(4)] \left[\min((1, 1, 0, 0.5, 0.5, 0.5)^T(A), 1)\right] \tag{86}
+ \min((0, 1, 1, 0.5, 0.5, 0.5)^T(A), 1) + \min((0.5, 0.5, 0.5, 1, 1, 0)^T(A), 1) \tag{87}
+ \min((0.5, 0.5, 0.5, 1, 1, 0)^T(A), 1) + \min((0.5, 0.5, 0.5, 1, 0, 1)^T(A), 1) \tag{88}
+ \min((0.5, 0.5, 0.5, 1, 0, 1)^T(A), 1) \tag{89}
$$

where $(x_a, x_b, x_c, x_d, x_e, x_f)^T$ is a modular function with elements $x_a, x_b, x_c, x_d, x_e, and x_f$. Hence, if all coefficients are non-negative, then $g$ is an SCMM (in fact, $g$ is a sum of weighted cardinality truncations, defined in Lemma 5.10). The non-negativity of the coefficients holds whenever the inequalities stated in the theorem are met. The “only if” part of the theorem is more involved and thus is given in Appendix A.

6.2 The DSF Family Grows Strictly with the Number of Layers

It is clear that a k-layer DSF can easily express a $k - 1$ layer DSF simply by using a linear function at the final unit. Hence, if we say that DSF$_k$ is the family of all deep submodular functions with $k$ layers, we have that DSF$_{k-1} \subseteq$ DSF$_k$. It is also clear that DSF$_0 \subset$ DSF$_1$ since DSF$_0$ are modular functions while DSF$_1$ are SCMMs. In the previous section, we demonstrated by example that DSF$_1 \subset$ DSF$_2$.

In this section, we show that DSFs become strictly more capable as the allowable number of layers increases, meaning there are $k$-layer functions that cannot be represented with $k - 1$ layers, and hence DSF$_{k-1} \subset$ DSF$_k$ for any $k$. This result is similar to some of the recent results from the DNN literature where it is shown that in some cases, it would require exponentially many hidden units to implement a network with more layers [40]. In the DSF case, however, we show that in some cases, there is no way to represent certain $k$-layer DSFs with a $k - 1$ layer function, which means that the class of DSFs is strictly increasing with the number of layers. This is different than standard neural networks where it is shown that even a shallow neural network is a universal approximator [61]. In order to do this in the DSF case, however, we allow the ground set correspondingly to grow in size with the number of layers.

We begin with a number of definitions and prerequisite lemmas.

**Definition 6.6 ((A, B, C)-function).** We say that polymatroid function $f$ is an (A, B, C)-function if $A, B, C \subseteq V$ are three non-empty disjoint subsets of $V$ and where $f$ satisfies the following:

$$
f(A \cup B \cup C) = f(A \cup B) = f(B \cup C) = f(C \cup A) = f(A) + f(B) = f(B) + f(C) = f(C) + f(A) \tag{90}
$$

**Definition 6.7 (strong (A, B, C)-function).** We say that $f$ is a strong (A, B, C)-function if $f$ is an (A, B, C)-function and if $f(A \cup B \cup C) > 0$.

**Lemma 6.8.** If $f$ is an (A, B, C)-function, then $f(A) = f(B) = f(C)$. If $f$ is a strong (A, B, C)-function, then $f(A) = f(B) = f(C) > 0$.

**Proof.** $f(A) + f(B) = f(B) + f(C) = f(C) + f(A)$ implies $f(A) = f(B) = f(C)$. If $f$ is strong, we have $f(A \cup B \cup C) > 0$. Therefore, $f(A) = \frac{1}{2} f(A \cup B \cup C) > 0$.  

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Figure 5: Example cycle matroids whose rank functions are in $F_k$. On the left we have $k = 1$ so $|V| = 3$ where the example shows a cycle matroid on a graph which is just a three-cycle. In the middle we have $k = 2$ so $|V| = 9$, where $V_1 = \{a,d,e\}$, $V_2 = \{b,f,g\}$, and $V_3 = \{c,h,i\}$. The figure shows a cycle matroid rank where each group $V_i$ is itself a three cycle. On the right shows an example with $k = 3$, $|V| = 27$ where $V_i$ for $i \in \{1,2,3\}$ is a set of nine elements, and $V_{ij}$ for $i,j \in \{1,2,3\}$ is a set of three elements comprising a three-cycle. These examples demonstrate that $F_k$ is non-empty.

A simple example of such a function is a cycle matroid rank function with $A = \{a\}$, $B = \{b\}$, and $C = \{c\}$, where $\{a,b,c\}$ are the edges of a 3-cycle in the cycle matroids associated graph. Note that in any $(A,B,C)$-function, we have $I_f(A;B) = I_f(B;C) = I_f(C;A) = 0$. In a strongly $(A,B,C)$-function, we have $I_f(A;B,C) > 0$. Hence, these functions have no interaction between any two groups but there is a three-way interaction amongst the three groups. Like surplus being zero, $(A,B,C)$-function that are mixtures force properties amongst the components.

**Lemma 6.9.** If $f = \sum_{i=1}^m f_i$ is an $(A,B,C)$-function, then $f_i$ is an $(A,B,C)$-function for all $i$.

**Proof.** First, conditioning on the pair $A,B$, since $\sum_{i=1}^m f_i(A \cup C) = f(A \cup C) = 0$ and $f_i(A \cup C) \geq 0$ for each $i$, we have $f_i(A \cup C) = 0$ for each $i$. Doing the same for pair $B,C$ and $C,A$, we have $f_i(A \cup B) = f_i(B \cup C) = f_i(C \cup A) = f_i(A \cup B \cup C)$.

Next, since $\sum_{i=1}^m f_i(A) + f_i(B) - f_i(A \cup B) = f(A) + f(B) - f(A \cup B) = 0$ and $f_i(A) + f_i(B) - f_i(A \cup B) \geq 0$ for all $i$, we have $f_i(A) + f_i(B) = f_i(A \cup B)$ for all $i$. Doing the same for pairs $B,C$ and $C,A$ yields the result.

**Definition 6.10.** Given a function $f : 2^V \to \mathbb{R}$, and a subset $V' \subseteq V$, define the restricted function $f_{V'} : 2^{V'} \to \mathbb{R}$ as $f_{V'}(X) = f(X)$ for all $X \subseteq V'$.

A restricted function $f_{V'}(X)$ has a restricted ground set, and by stating $f_{V'}(X)$ we assume $X \subseteq V'$.

**Lemma 6.11.** Let $h$ be polymatroidal, $\phi$ be normalized monotone non-decreasing concave, and define $h(X) = g(X) + m_\pm(X)$, where $g(X) = \phi(h(X))$. If $g$ is a strongly $(A,B,C)$-function, then $h_D(X) = \gamma h(X) + m_\pm(X)$ for $D = A \cup B$, $D = B \cup C$, and $D = C \cup A$.

**Proof.** Since $g$ is strongly $(A,B,C)$, we have $I_g(A;B) = 0$, while $g(A) = g(B) > 0$, which by Lemma 5.32 means that $\alpha$, the last linear point of $\phi$, must be no less than $h(A,B)$. Hence, for any $X \subseteq A \cup B$, $h(X) = \gamma h(X) + m_\pm(X)$ for some $\gamma > 0$. The same holds true for $B \cup C$ and $C \cup A$.

Given $k \geq 1$ and a ground set $V$ where $|V| = 3^k$, we name each element $v \in V$ as $v_{a_1,a_2,...,a_k}$ where $a_i \in \{1,2,3\}$ for $i = 1,2,...,k$. Define $V_{a_1,a_2,...,a_k} \cup V_{a_1,a_2,...,a_j}$ for $1 \leq j \leq k - 1$, define $V_{a_1,a_2,...,a_j} = V_{a_1,a_2,...,a_j,1} \cup V_{a_1,a_2,...,a_j,2} \cup V_{a_1,a_2,...,a_j,3}$. For example, $V = V_1 \cup V_2 \cup V_3$, $V_1 = V_{11} \cup V_{12} \cup V_{13}$, $V_2 = V_{21} \cup V_{22} \cup V_{23}$, $V_{11} = V_{111} \cup V_{112} \cup V_{113}$, and so on.

**Definition 6.12.** We define $F_k$ as the set of set functions $f : 2^V \to \mathbb{R}$ where $|V| = 3^k$, $f(V) > 0$ and $f$ is a $(V_{a_1,a_2,...,a_j,1},V_{a_1,a_2,...,a_j,2},V_{a_1,a_2,...,a_j,3})$-function for all $a_i \in \{1,2,3\}$, $1 \leq i \leq j$, and $0 \leq j \leq k - 1$.

We also define $F_k$ as the set of set functions $f : 2^V \to \mathbb{R}$ where $|V| = 3^k$, and $f$ is a strongly $(V_{a_1,a_2,...,a_j,1},V_{a_1,a_2,...,a_j,2},V_{a_1,a_2,...,a_j,3})$-function for all $a_i \in \{1,2,3\}$, $1 \leq i \leq j$, for all $0 \leq j \leq k - 1$. 

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Figure 5 shows three examples of cycle matroids whose ranks are in $F_k$ for $k = 1, 2, 3$ thus demonstrating that $F_k$ is non-empty. To show that there are DSFs who are members of $F_k$, consider the following example.

**Example 6.13.** Define $\hat{f}_k : 2^{V_k} \to \mathbb{R}$, where $|V_k| = 3^k$. Define $\hat{f}_1(X) = \frac{1}{2} \min(|X|, 2)$. For $k \geq 2$, $V_k$ is partitioned into three sets $V_{k1}$, $V_{k2}$, and $V_{k3}$ where $|V_{k1}| = |V_{k2}| = |V_{k3}| = 3^{k-1}$. The level-$k$ function is defined as $\hat{f}_k(X) = \frac{1}{2} \min(\sum_{i=1,2,3} \hat{f}_{k-1}(X \cap V_{ki}), 2)$.

Hence, $\hat{f}_k$ is like a $[0,1]$-normalized laminar matroid rank function with the laminar family of sets $F_k = \{V_k, V_{k1}, V_{k2}, V_{k3}, V_{k11}, V_{k12}, V_{k13}, V_{k21}, \ldots\}$. An immediate consequence is the following.

**Lemma 6.14.** $\hat{f}_k \in F_k$ and $\hat{f}_k$ can be expressed as a $k$-layer DSF.

We also note that the families $F_k$ and $F_k'$ are the same.

**Lemma 6.15.** $F_k' = F_k$

**Proof.** Immediately, we have $F_k \subseteq F_k'$

To show the other direction, assume there exists $f \in F_k'$ and $v \in V$ such that $f(v) = 0$ where $v$ is labeled as $v_{a_1,a_2,\ldots,a_k}$. Then we have $f(V_{a_1,a_2,\ldots,a_{k-1}}) = 2 \times f(V_{a_1,a_2,\ldots,a_{k-1},a_k}) = 0$, $f(V_{a_1,a_2,\ldots,a_{k-2},a_{k-1}}) = 2 \times f(V_{a_1,a_2,\ldots,a_{k-2},a_{k-1},a_k}) = 0$, and so on until finally we have $f(V) = 0$ which contradicts with the definition of $F_k'$. Hence, for all $f \in F_k'$ and $v \in V$, we have $f(v) > 0$ and by monotonicity $f(A) > 0$ for all $A$. Therefore, $f \in F_k$ and $F_k' \subseteq F_k$.

**Lemma 6.16.** Given $f \in F_k$, suppose that $f = \sum_{i=1}^{m} f_i$. If $f_i(V) > 0$, then $f_i \in F_k$ for all $i$.

**Proof.** This is immediate when considering lemmas 6.9 and 6.15.

**Lemma 6.17.** Given $f \in F_k$, we have $\gamma f \in F_k$ for all $\gamma > 0$. If $k \geq 2$, we have $f_{V_i} \in F_{k-1}$, for $i \in \{1, 2, 3\}$, where $V_i$ is defined in Definition 6.12.

**Proof.** This is immediate from the definitions.

**Lemma 6.18.** For all $f \in F_k$ and $\phi$ be a normalized monotone non-decreasing concave function. If $f = \phi(f')$, then $f_{V_i} \in F_{k-1}$, for $i \in \{1, 2, 3\}$.

**Proof.** Using Lemma 6.11, we have $f_{V_i} = \gamma f_{V'}$, where $\gamma > 0$ is a constant. Also we have $f_{V_i} \in F_{k-1}$ according to second part of lemma 6.17. So $f_{V_i}' \in F_{k-1}$ according to first part of lemma 6.17.

For any $f \in F_k$, we have that $f(v|V \setminus \{v\}) = 0$ which follows since if $v = v_{a_1,a_2,\ldots,a_{k-1},1}$, $v' = v_{a_1,a_2,\ldots,a_{k-1},2}$, and $v'' = v_{a_1,a_2,\ldots,a_{k-1},3}$, $0 = f(v|v',v'') \geq f(v|V \setminus \{v\}) \geq 0$. Hence, all members of $F_k$ are totally normalized in this sense [31, 30].

As mentioned in Section 4, a DSF allows for the use of an arbitrary final modular function $m_\pm$ at the top layer. If it is the case that a given $f \in F_k$ is represented as a DSF, since $f$ is totally normalized and since the polymatroidal part must have non-negative gain, the final $m_\pm$ must be non-positive as otherwise we would have $f(v|V \setminus \{v\}) > 0$. Hence, in order to show that a given $f \in F_k$ can not be represented by a DSF with fewer than $k$ layers, it is sufficient to show that a function of the form $f + m_+$, where $f \in F_k$ and $m_+$ is a non-negative modular function, can not be expressed as a $k-1$ layer DSF having $m_+ = 0$. To this end, we introduce the following class:

**Definition 6.19.** We define the class of functions $G_k = \{f + m_+ | f \in F_k, m_+ \in M_+\}$ where $M_+$ is the set of all non-negative normalized modular functions.

The addition of a modular function to an $f \in F_k$ does not change any surplus. Hence, for a $g \in G_k$ with $g = f + m_+$ with $f \in F_k$, we have that $I_g(A;B) = I_f(A;B)$ for any disjoint sets $A, B$, and that $S_g(A) = S_f(A)$ for any set $A$. 

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The properties of total normalization \([31, 30]\) will be further useful in the below, so we define functional operators that totally normalize a given function. Define the functional operator \(\mathcal{M} : (2^V \to \mathbb{R}) \to (V \to \mathbb{R})\) that maps from submodular functions to a modular function as follows, for all \(A \subseteq V\):

\[
(\mathcal{M}f)(A) = \sum_{a \in A} f(a|V \setminus \{a\}).
\]

Hence, \(\mathcal{M}f\) is a modular function consisting of elements which are the smallest possible gain given by submodular \(f\). We also define a total normalization functional operator \(\mathcal{T} : (2^V \to \mathbb{R}) \to (2^V \to \mathbb{R})\) as follows:

\[
(\mathcal{T}f)(A) = f(A) - (\mathcal{M}f)(A).
\]

Then clearly \(\mathcal{T}f\) is a polymatroid function that is totally normalized (i.e., \((\mathcal{T}f)(v|V \setminus \{v\}) = 0\)), and we have the identity \(f = \mathcal{T}f + \mathcal{M}f\), meaning that any submodular function can be decomposed into a totally normalized polymatroid function plus a modular function \([31, 30]\). The decomposition is unique because if \(f = f' + m\) where \(f'\) is any function having \(f'(v|V \setminus \{v\}) = 0\), then \(f(v|V \setminus \{v\}) = m(v)\) so we must have that \(m = \mathcal{M}f\).

The operator \(\mathcal{T}\) is linear, \(\mathcal{M}(f_1 + f_2) = \mathcal{M}f_1 + \mathcal{M}f_2\), as is \(\mathcal{T}\). Also, in the present case, since \(f\) is presumed polymatroidal, the modular function is non-negative, i.e., \((\mathcal{M}f)(v) \geq 0\) for all \(v\).

The next lemma states that if \(f\) is representable as a sum, then each term must either be a member of \(G_k\) or must be purely a non-negative modular function.

**Lemma 6.20.** Given \(f \in G_k\), suppose that \(f = \sum_{i=1}^l f_i\). Then \(f_i \in G_k \cup M_+\) for all \(i\). Furthermore, for at least one \(i\), we have \(f_i \in G_k\).

**Proof.** Consider \(\mathcal{M}f = \mathcal{M} \sum_{i=1}^l f_i = \sum_{i=1}^l \mathcal{M}f_i\) and \(\mathcal{T}f = \mathcal{T} \sum_{i=1}^l f_i = \sum_{i=1}^l \mathcal{T}f_i\). For any \(h \in F_k\) and \(m \in M_+, \mathcal{M}(h + m) = m\), and hence \(\mathcal{T}f = f - \mathcal{M}f \in F_k\). Thus, by Lemma 6.16, we have either that \(\mathcal{T}f_i\) is identically zero or is otherwise an element of \(F_k\). Hence, when considering that \(f_i = \mathcal{M}f_i + \mathcal{T}f_i\), if \(\mathcal{T}f_i\) is zero, \(\mathcal{M}f_i + \mathcal{T}f_i \in M_+\) and if not \(\mathcal{M}f_i + \mathcal{T}f_i \in G_k\). Furthermore, since \(f \in G_k\) we can not have that for all \(i\), \(f_i \in M_+\).

**Lemma 6.21.** Given an \(f \in G_k\), if \(f = \phi(f')\), where \(\phi\) is normalized non-decreasing concave, and \(f'\) is polymatroidal, then \(f'_i \in G_{k-1}, i \in \{1, 2, 3\}\).

**Proof.** Since \(f \in G_k\), we have that we have \(I_f(V_i|V_j) = 0\), for \(i, j \in \{1, 2, 3\}, i \neq j\), while \(g(V_i) = g(V_j) > 0\). This, Lemma 5.32, means that \(\alpha\), the last linear point of \(\phi\), must be no less than \(f'(V_i|V_j)\). Hence, \(f'_i = \gamma f'_i\) for \(i \in \{1, 2, 3\}\) and for some constant \(\gamma > 0\).

Since \(f = \mathcal{M}f + \mathcal{T}f\) and \(f \in G_k\), \(\mathcal{T}f \in F_k\) and \(\mathcal{M}f \in M_+\). Thus, \((\mathcal{T}f)_i \in F_k\) by Lemma 6.17, and we also have that \((\mathcal{M}f)_i \in M_+\). Hence, since \(f = \mathcal{T}f + \mathcal{M}f\) for any \(X \subseteq V\), we have \(f'_i = \frac{1}{\gamma}(\mathcal{M}f)_i + (\mathcal{T}f)_i \in G_{k-1}\).

**Theorem 6.22.** Any \(f \in G_k\) can not be expressed via a \((k-1)\)-layer DSF having \(m_+ = 0\).

**Proof.** We prove this by induction.

To establish the base case, all \(f \in G_1\) can not be expressed via a 0-layer DSF since a 0-layer DSF is modular while any \(f \in G_1\) is not modular since there are sets that have strictly positive surplus. Hence, the induction step assumes that any \(f \in G_{k-1}\) can not be expressed via a \((k-2)\)-layer DSF for \(k \geq 2\).

Next, suppose we find a \(f \in G_k\) where \(f\) can be expressed by a \((k-1)\)-layer DSF. Hence, we can express \(f = \phi(f')\) where \(\phi(\cdot)\) is concave and where \(f' = \sum_{i=1}^l f_i\). Since \(f\) is a \((k-1)\)-layer DSF, then for all \(i, f_i\) is a \((k-2)\)-layer DSF.

We may w.l.o.g., assume that \(f_i(V) > 0\) for all \(i\) (since if for any \(i\) we have \(f_i(V) = 0\), then it contributes nothing to the function for any \(A \subseteq V\) by monotonicity and non-negativity). By Lemma 6.21, we have that \(f'_i, f'_2, f'_3 \in G_{k-1}\). For \(j \in \{2, 3\}\), we have that \(f'_j = \sum_{i=1}^l f_i V_j\), and by Lemma 6.20, for all \(i = 1, 2, \ldots, m\) and \(j \in \{1, 2, 3\}\), we have that \(f_i V_j \in G_{k-1} \cup M_+\). Also, for each \(j \in \{1, 2, 3\}\), there is at least one \(i\) where \(f_i V_j \in G_{k-1}\). For these instances, by the induction step, \(f_i V_j\) can not be expressed in \((k-2)\)-layer DSF. Since \(f_i\) is more complex than \(f_i V_j\), \(f_i\) also can not be expressed using a \((k-2)\)-layer DSF, which contradicts the above statement that \(f_i\) is a \((k-2)\)-layer DSF.

Hence, we can not find an \(f \in G_k\) that can be expressed as a \((k-1)\)-layer DSF.
Theorem 6.23. There are \( k \)-layer DSFs that cannot be expressed using \( k' \)-layer DSFs for any \( k' < k \).

Letting \( DSF_k \) be the family of \( k \)-layer DSFs, it is interesting to consider what happens with \( \lim_{k \to \infty} DSF_k \). To show the above result, we needed for the ground set to grow exponentially with \( k \) which means that for the flexibility of DSFs to grow, we need an ever increasing ground set. It remains an open question to determine if, when the ground set size is constant and fixed, if \( DSF_k \) comprises a larger family, or if expressing certain DSF\(_k\)s with \( k - 1 \) layers requires an exponential number of hidden units, analogous to \([40]\).

### 6.3 The Family of Submodular Functions is Strictly Larger than DSFs

Our next result shows that, while DSFs are richer than SCMMs, and the DSF family grows with the number of layers, they still do not encompass all polymatroid functions. We show this by proving that the cycle matroid rank function on \( K_4 \) is not achievable with DSFs. We adopt the idea of the backpropagation style proof in Lemma 5.18 and utilize the form of DSF given in Eqn. (11) where we strip off the DSF layer-by-layer until we reach a one-layer DSF that, as is shown, is unable to represent a cycle matroid rank over \( K_4 \). In particular, we backpropagate a necessary lack of surplus, a required linearity, and also a required pairwise surplus, from the root down to the very first layer. This shows that, for up to size three sets, the DSF must be similar to a mixture of concave over modular, and which then is unable to maintain a pairwise surplus necessary for the cycle matroid rank function.

The reader is encouraged to review the notation in Equation (11). We start with a number of lemmas that culminate in Theorem 6.26.1.

By applying Lemma 5.20 and Theorem 5.24 recursively according to a DSF’s DAG, there are some important and powerful implications for DSF with positive weights. Firstly, if we ever find an internal network node and corresponding set in surplus, it means some surplus is preserved all the way to the root. Correspondingly, any set \( A \) not in surplus by the network as a whole must not be in surplus at any internal node. This allows us to place constraints at one part of the network to cause consequences at distant points (i.e., many layers away) elsewhere in the network. For a DSF (or SCMM), once a node is in surplus, there is no way to recover anywhere else in the network (since there are no zero weights). We formalize this in the following:

**Corollary 6.23.1 (Preservation of Surplus).** If \( \mathcal{S}_v(A) > 0 \) for some internal node \( u \) in the DSF, then \( \mathcal{S}_v(A) > 0 \) where \( v \) is a higher node (closer to the root \( v \)). In other words, if there is no surplus at the higher node \( v \) for some \( A \), there can be no surplus at any lower internal node in a DSF. This is also true for grouped surplus (Definition 5.26).

This result immediately follows Theorem 5.24. This means that zero surplus at the root \( \mathcal{S}_v(A) = 0 \) on a set \( A \) means all internal nodes must also have zero surplus on \( A \). For an SCMM, it means that if one term is in surplus then the sum must also be in surplus. This is a crucial result used in Theorem 6.26.1.

**Corollary 6.23.2 (Modular on 3-Cycle).** Let \( f : 2^V \to \mathbb{R} \) be a DSF in the above form using the above notation, and assume \( f(A) = r(A) \) where \( r \) is a cycle matroid rank function over the edges of \( K_4 \). Then for any \( v \in V \) and any 3-cycle \( C = \{a, b, c\} \) having \( g_v(a) = \psi_v(1_a) = 0 \), then \( \mathcal{S}_v(\{a, b, c\}) = 0 \) (i.e., \( g_v \) is modular at the cycle \( C \)).

**Proof.** This follows immediately from Lemma 5.31 where the three cycle consists of edges \( \{a, b, c\} \) with \( A = \{a\}, B = \{b\}, C = \{c\}, \) and \( h = g_v \) which must be polymatroidal in a DSF for any \( v \in V \).

**Lemma 6.24 (Linear Part of Hidden Units).** Let \( f : 2^V \to \mathbb{R} \) be a DSF in the above form using the above notation, and assume \( f(A) = r(A) \) where \( r \) is a cycle matroid rank function over the edges of \( K_4 \). We are given any \( v \in V \), any 3-cycle \( C = \{a, b, c\} \), and any \( e' \notin C \) having \( g_v(e') > 0 \), \( g_v(C) > 0 \), and \( I_{g_v}(e'; C) = 0 \). Then any surplus \( \mathcal{S}_v(C) > 0 \) given to \( C \) is not due to any non-linearity in \( \phi_v(\cdot) \) and instead is caused by \( \phi_v(\cdot) \).

**Proof.** Thus, since \( w_{uv} \geq 0 \) for all \( u \in pa(v) \setminus V \), and the modular part of \( \phi_v \) does not change pairwise surplus, we may apply Lemma 5.32 with \( g(X) = g_v(X), h(X) = \phi_v(1_X), A = \{e'\}, \) and \( B = C \), which means the linear range of \( \phi_v \) must include \([0, \phi_v(1_C) + \phi_v(1_e)]\).
Lemma 6.25 (Decomposition of sets of three-cycles). Let $f : 2^V \to \mathbb{R}$ be a DSF in the above form using the above notation, and assume $f(A) = r(A)$ where $r$ is a cycle matroid rank function over the edges of $K_4$. We are given any $v \in V$, and a subset $cid(v) \subseteq \{1, 2, 3, 4\}$ of indices of the four three-cycles $(C_1, C_2, C_3, \text{ and } C_4)$ of the matroid where $|cid(v)| \geq 2$ and where the following is true:

1. For $i \in cid(v)$, $g_v(C_i) > 0$,
2. for $e \in \bigcup_{i \in cid(v)} C_i$, $g_v(e) > 0$,
3. for $e \notin \bigcup_{i \in cid(v)} C_i$, $g_v(e) = 0$,
4. and for $i \in cid(v)$, 3-cycle $C_i$ and $e \in C_i$, we have $I_{g_v}(e; C_i \setminus \{e\}) = g_v(e) - g_v(e|C_i \setminus \{e\}) = g_v(e)$.

Then we may for all $X$ of size up to three write $g_v(X)$ as

$$g_v(X) = \sum_{u \in U} w_u g_u(X)$$

with $w_u \geq 0$ and where for all $u \in U = pa(v) \setminus V$, there is a set of cycle indices $cid(u) \subseteq cid(v)$ having:

1. For $i \in cid(u)$, $g_u(C_i) > 0$,
2. for $e \in \bigcup_{i \in cid(u)} C_i$, $g_u(e) > 0$,
3. for $e \notin \bigcup_{i \in cid(u)} C_i$, $g_u(e) = 0$,
4. and for $i \in cid(u)$, 3-cycle $C_i$ and $e \in C_i$, we have $I_{g_u}(e; C_i \setminus \{e\}) = g_u(e) - g_u(e|C_i \setminus \{e\}) = g_u(e)$.

If $u$ is a first-layer hidden unit in the DSF then $|cid(u)| = 1$.

Proof of Lemma 6.25. For clarity, we offer the proof as a series of numbered statements.

1. $g_v(\cdot)$ has to be modular on any set up to size two, as otherwise an unrecoverable surplus will occur by Corollary 6.23.1. This means that $\phi_v$ has to be linear up to any valuation of any size two set (i.e., $\varphi_v(1_X)$ is still in the linear part of $\phi_v(\cdot)$ for any $X$ with $|X| = 2$).

2. For the same reason, the nonlinear part of $\phi_v(\cdot)$ must not start before the valuation $\varphi_v(1_X)$ for any $X$ with $|X| = 3$ not in surplus (i.e., with $\mathcal{G}_v(X) = 0$, any matroid independent set of size three).

3. Since $|cid(v)| \geq 2$, for any $i,j \in cid(v)$, corresponding three-cycles $C_i,C_j$ and any element $e' \in C_j$ where $e' \notin C_i$, we have by Corollary 6.23.1 that

$$I_{g_v}(e'; C_i) = g_v(e') - g_v(e'|C_i) = 0.$$  

(95)

Therefore, since $g_v(e') > 0$ and $g_v(C_i) > 0$, by Lemma 6.24 the non-linear part of $\phi_v$ must not start before the valuation $\varphi_v(1_{C_i})$ for any $i \in cid(v)$.

4. For any $i \notin cid(v)$, $\exists e \in C_i$ with $g_v(e) = 0$. By Corollary 6.23.2, this means $g_v$ is modular at $C_i$.

5. Considering the two previous statements, the non-linear part of $\phi_v(\cdot)$ must not start before the valuation $\varphi_v(1_X)$ for any set with $|X| = 3$. Since such an $X$ is still in the linear part of $\phi_v$ we may write $g_v(\cdot)$ as:

$$g_v(X) = \alpha_v \varphi_v(1_X) = \sum_{u \in pa(v) \setminus V} \alpha_v w_{uv} \psi_u(1_X) + \alpha_v (m_v, 1_X)$$

(96)

for any $X$ up to size three, for some appropriate positive constant $\alpha_v \in \mathbb{R}_+$. 

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6. We are given that for any \( i \in \text{cid}(v) \), 3-cycle \( C_i \), and any \( e \in C_i \),

\[
I_{g_u}(e; C_i \setminus e) = g_u(e) - g_u(e|C_i \setminus \{e\}) = g_u(e) > 0. \tag{97}
\]

From the previous statements, however, the surplus of any such 3-cycle is not addressed by any non-linearity in \( \varphi \), and must instead be handled by \( \varphi \), which, since \( g_u(e) > 0 \), means that

\[
0 = g_u(e|C_i \setminus \{e\}) = \sum_{u \in \text{pa}(v) \setminus V} \alpha_u w_{uv} \varphi_u(1_e | 1_{C_i \setminus \{e\}}) + m_u(e) \tag{98}
\]

Since \( \psi_u(1_e | 1_{C_i \setminus \{e\}}) \geq 0 \), for all \( u \in \text{pa}(v) \setminus V \), this requires \( 0 = \psi_u(1_e | 1_{C_i \setminus \{e\}}) = g_u(e|C_i \setminus \{e\}) \). Since \( m_u(e) \geq 0 \), this also implies that \( m_u(e) = 0, \forall e \in C_i \). Since \( g_u(e) = 0 \) for \( e \notin \cup_{i \in \text{cid}(v)} C_i \), we have that \( m_u(e) = 0, \forall e \in V \). Hence, the above establishes that for all \( u \in \text{pa}(v) \setminus V \):

\[
I_{g_u}(e; C_i \setminus \{e\}) = g_u(e) - g_u(e|C_i \setminus \{e\}) = g_u(e) \tag{99}
\]

Next we need to consider whether \( g_u(e) = 0 \) or not.

7. If there is a \( u \in \text{pa}(v) \setminus V \) and corresponding \( i \in \text{cid}(v) \), 3-cycle \( C_i \) having \( \psi_u(1_e) = 0 \) for some \( e \in C_i \), then Lemma 6.23.2 means that \( \psi_u() \) must be modular at \( C_i \). But then we must have \( \psi_u(1_e') = 0 \) for \( e' \in C_i \) otherwise, by modularity, we’d get \( \psi_u(1_e'|1_{C_i \setminus \{e'\}}) = \psi_u(1_{e'}) > 0 \) violating the requirement of Equation (98).

8. Thus, this means that for every \( u \) and every \( i \in \text{cid}(v) \) and 3-cycle \( C_i \), we have either \( \forall e \in C_i, \psi_u(1_e) = 0 \) or alternatively \( \forall e \in C_i, \psi_u(1_e) > 0 \), and in this latter case \( u \) must give \( C_i \) a positive surplus (to satisfy Equation (99)). Any \( u \) giving no surplus to any of the 3-cycles in \( \text{cid}(v) \) thus must have \( \forall e \in V, \psi_u(1_e) = 0 \) and so can be removed from the network without effect (which we assume in the below).

9. Hence, for all \( u \) there exists a set \( \text{cid}(u) \subseteq \text{cid}(v) \) where for all \( i \in \text{cid}(u) \), three-cycle \( C_i \), and \( e \in C_i \), we have \( g_u(e) > 0, g_u(C_i) > 0 \). For \( e \notin \cup_{i \in \text{cid}(u)} C_i \), \( g_u(e) = 0 \).

10. If \( u \) is one of the first layer hidden unit nodes, then \( g(A) = \phi_u(w_u(A)) \) is a simple concave over modular function \( w_u : V \rightarrow \mathbb{R}_+ \). Suppose that for this \( u \), we have \( |\text{cid}(u)| > 1 \), then taking \( i,j \in \text{cid}(u), i \neq j \), \( i,j \in \text{cid}(v) \), corresponding three-cycles \( C_i,C_j \) and any element \( e' \in C_i \) where \( e' \notin C_i \), we require by Corollary 6.23.1 that \( I_{g_u}(e'; C_i) = g_u(e') - g_u(e'|C_i) = 0 \). By Lemma 6.24, the non-linear part of \( \phi_u \) must not start before the valuation of \( w_u(C_i) \), meaning \( \phi_u(w_u(C_i)) \) is modular on the cycle, contradicting Equation (98). Hence, we must have \( |\text{cid}(u)| = 1 \) for first layer hidden nodes.

\[\blacksquare\]

**Theorem 6.26** (DSFs are unable to represent the cycle matroid rank function on edges of \( K_4 \)).

**Proof.** Let \( f : 2^V \rightarrow \mathbb{R} \) be a DSF in the above form. We may, w.l.o.g., assume all weights are strictly positive, as the summations below will be based on \( u \in \text{pa}(v) \), so we assume that for all \( u \in \text{pa}(v), w_{uv} > 0 \).

Consider, in Eqn. (11) , the top layer concave function along with the arbitrary modular function, and suppose that \( f(A) = \psi(A) + m(A) = r(A) \) for all \( A \) where \( r : 2^V \rightarrow \mathbb{Z}_+ \) is a cycle matroid rank function on \( K_4 \). Hence, \( g(A) = \psi(A) = r(A) - m(A) \) which is an assuredly polymatroidal part of \( f(A) \).

Let \( C_1, C_2, C_3, \) and \( C_4 \) be the four three-cycles of the matroid. Note that for all \( i \), we have \( J_f(C_i) > 0 \) for all \( i \), and \( f(C_i) > 0 \). Also, for all \( e \in V, f(e) > 0 \). Hence, define \( \text{cid}(\hat{\mathcal{S}}) = \{1, 2, 3, 4\} \). By Theorem 6.25, for any set \( X \) with \( |X| \leq 3 \), we may write \( g_\hat{\mathcal{S}}(X) \) as follows:

\[
g_\hat{\mathcal{S}}(X) = \sum_{u \in U} w_u g_u(X) \tag{100}
\]

where \( \text{cid}(u) \subseteq \text{cid}(\hat{\mathcal{S}}) \), and where for all \( u \in U, i \in \text{cid}(u) \), we have \( g_u(C_i) > 0 \), \( g_u(e) > 0 \) for \( e \in \cup_{i \in \text{cid}(u)} C_i \), and \( g_u(e) = 0 \) for \( e \notin \cup_{i \in \text{cid}(u)} C_i \). Hence we may write \( g_\hat{\mathcal{S}}(X) \) as:

\[
g_\hat{\mathcal{S}}(X) = \sum_{u \in U: |\text{cid}(u)| = 1} w_u g_u(X) + \sum_{u \in U: |\text{cid}(u)| > 1} w_u g_u(X) \tag{101}
\]

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For any $u \in U$ with $\text{cid}(u) > 1$, by Theorem 6.25, we may, for any set $X$ of size $|X| \leq 3$, write it as:

$$g_u(X) = \sum_{u' \in U'} w_{u'} g_{u'}(X)$$

(102)

where $\text{cid}(u') \subseteq \text{cid}(u)$. Thus, we have

$$g_s(X) = \sum_{u \in U : \text{cid}(u) = 1} w_u g_u(X)$$

(103)

$$+ \sum_{u' \in U' : \text{cid}(u') = 1} w_{u'} g_{u'}(X) + \sum_{u' \in U' : \text{cid}(u') > 1} w_{u'} g_{u'}(X)$$

(104)

This process may continue recursively, applying Theorem 6.25 each time, until we reach all units in the bottom layer of the DSF. We are guaranteed termination since the DSF is itself finite size. Also, since the bottom layer consists of single concave composed with modular functions, all have $\text{cid}() = 1$. Hence, for $X$ with $|X| \leq 3$, the entire DSF can be expressed as:

$$g_s(X) = \sum_{u \in U^{(l)}} w_u g_u(X)$$

(105)

where $\text{cid}(u) = 1$ and where we may partition $U^{(l)}$ in to four disjoint sets corresponding to the four cycles, where in each index set we have surplus only of one of the cycles. This means that it is not possible to achieve, for a cycle $C$ and $e \in C$,

$$I_{g_s}(e; C \setminus \{e\}) = g_s(e) - g_s(e|C \setminus \{e\}) = g_s(e) = 1$$

(106)

since some of the terms in the sum are non-zero meaning $g_s(e|C \setminus \{e\}) > 0$, thus contradicting that $f(X) = r(X)$ for all $X \subseteq V$.

The above results therefore imply the following.

**Corollary 6.26.1 (SCCMs ⊂ DSFs ⊂ Submodular Functions).** The family of SCCMs is smaller than that of DSFs, and the family of DSFs is smaller than the family of all submodular functions. That is, let $C_n$ be the set of all submodular functions over ground set $V$ of size $n$ and let $\text{DSF}_k$ be the family of DSFs with $k$ layers on $V$, and $\text{SCCM}$ be the family of SCCMs on $V$ with an arbitrary number of component functions. Then, for any $k$, $\text{SCCM} \subset \text{DSF}_k \subset C_n$.

While DSFs do not comprise all submodular functions, a consequence of Theorem 5.12 is that the input to a DSF can be any set of polymatroid functions. Let $f$ be a DSF with $k$ inputs and a ground set $V = \{1, 2, \ldots, k\}$. Then we can consider the standard way to utilize a DSF, in the context of Theorem 5.12, as one where the $i$th input is a function $g_k(A) = 1_{k \in A}$ which is modular. Theorem 5.12 allows for any polymatroid function to be used as input to a DSF, not just an indicator function, and hence the DSF can be used to add interactions between and perhaps improve these functions in some way. Hence, if several of the $g_k$ are cycle matroid rank functions, and if the DSF is learnt, the resulting family is expanded to include at least those matroid ranks used as input. It remains an open question to see if there is a small finite fixed set of input polymatroid functions that can be cascaded into a DSF in order to achieve all submodular functions.

It is also worth noting that in [163] it is shown that the entropy function $f(A) = H(X_A)$ when seen as a set function must satisfy inequalities that are not required for an arbitrary polymatroid function, thus implying that entropy also does not comprise all submodular function. An additional open problem, therefore, is to compare the family of DSFs to that of entropy functions.

### 7 Applications in Machine Learning and Data Science

In this section, we describe a number of possible DSF applications in machine learning and data science.
7.1 Learning DSFs

As mentioned in Section 1, recent studies [52, 11, 43, 42] show that learning submodular functions can be easier or harder depending on the learning setting.

A general outline of various learning settings is given in [76, 43] — here, we give only a very brief overview. To start, learning may involve several families of functions $F, H,$ and $T$ members of which are mappings from $2^V$ to $\mathbb{R}$. There is some true function $f \in F$ to be learnt based on information obtained via samples of the form $(A, f(A))$ for $A \subseteq V$. One wishes to produce an approximation $\hat{f} \in H$ to $f$ that is good in some way.

Learning submodular functions has been studied under a number of possible variants. For example, there is typically a probability distribution $\text{Pr}$ over subsets of $V$ (i.e., $\text{Pr}(S = A) \geq 1$ and $\sum_{A \subseteq V} \text{Pr}(S = A) = 1$ where $S$ is a random variable). A set of samples $D = \{(A_i, f(A_i))\}_{i}$ is obtained via this distribution. The distribution $\text{Pr}$ might be unknown [11], or might be known (and in such case, might be assumed to be uniform [43, 42]). The quality of learning could be judged over all $2^n$ points or over some fraction, say $1 - \beta$, of the points, for $\beta \in [0, 1]$. In general, there is no specificity on the particular set of points, or the particular kind of points, that should be learnt as long as at least a (probability distribution measured) fraction $1 - \beta$ of them are learnt. Learning itself happens with some probability $1 - \delta$. I.e., there is some probability $\delta$ that the learning will not succeed. While learning asks for a function in $\hat{f} \in H$ that is good, we might judge $\hat{f}$ relative only to the best function $\tilde{f} \in T$ (the touchstone class). For example, in agnostic learning [76], we acknowledge that it might be difficult to show that learning is good relative to all of $F$ (say due to noise) but still feasible to show that learning is good relative to the best within $T$. Also, there are a variety of ways to judge goodness. In [11], goodness is judged multiplicatively, meaning for a set $A \subseteq V$ we wish that $f(A) \leq f(A) \leq g(n)f(A)$ for some function $g(n)$, and this is typically a probabilistic condition (i.e., measured by distribution $\text{Pr}$; goodness, or $f(A) \leq f(A) \leq g(n)f(A)$, should happen on a fraction at least $1 - \beta$ of the points). Alternatively, goodness may also be measured by an additive approximation error, say by a norm. I.e., defining $\text{err}_p(f, \hat{f}) = \|f - \hat{f}\|_p = (E_{A \sim \text{Pr}}[\|f(A) - \hat{f}(A)\|^p])^{1/p}$, we may wish $\text{err}_p(f, \hat{f}) < \epsilon$ for $p = 1$ or $p = 2$. In the PAC (probably approximately correct) model, we probably $(\delta > 0)$ approximately $(\epsilon > 0)$ or $(g(n) > 1)$ learn $(\beta = 0)$ with a sample or algorithmic complexity that depends on $\delta$ and $g(n)$. In the PMAC (probably mostly approximately correct) model [11], we also “mostly” $\beta > 0$ learn. In agnostic learning, $F \supseteq H = T$. Let $C_n$ be the space of all submodular functions. In some cases $F \supseteq C_n = H$ so we wish to learn the best submodular approximation to a non-submodular function. In other cases, $F = C_n \subseteq T \subseteq H$ meaning we are allowed to deviate from submodularity as long as the error is small.

In the machine learning community, $H$ may be a parametric family of submodular functions. For example, given a fixed set of component submodular functions, say $\{f_i\}_{i=1}^r$, one may wish to learn only the weights of a mixture $\{w_i\}$, to produce $f = \sum_i w_i f_i$, where $w_i \geq 0$ for all $i$ to ensure submodularity is preserved. What is learnt is only the coefficients of the mixture, not the components, so the flexibility of the family is determined by the diverseness and quantity of components used. Empirically, experiments that learn submodularity for various data science applications [140, 92], has been more successful than simply hand-designing a fixed submodular function. This is true both for image [150] and document [92] summarization tasks. There also has been some initial work on learnability bounds in [92]. Learning just the mixture coefficients of a mixture of submodular functions, while keeping the component functions themselves fixed, is only as flexible as the set of component functions allows, however. Given a small (or indiscriminately selected and hence potentially redundant) number of components, the family over which one can learn might be limited. As a result, one might need add a very large number of components before one obtains a sufficiently powerful family.

An alternative approach to learning a mixture that alleviates to some extent the above problem is to learn over a richer parametric family, and this is where DSFs hold promise. An approach to learning DSFs, therefore, is to learn within its parametric family, so $H = \text{DSF}_k$ for some finite $k$ and where $f_w \in \text{DSF}$ is parameterized by the vector $w$ that determines the topology (e.g., number and width of layers) of the network, the numeric parameters (set of matrices) within that topology, and the set of concave functions $\{\phi_u\}_u$. As shown in the present paper, DSFs represent a strictly larger family than SCMMs. Therefore, even in the mixture case above where the components may also be learnt, there are DSFs that are unachievable by SCMMs. In addition, by Theorem 5.12, a DSF rather than a mixture can be applied to a fixed set of input submodular components (e.g., some of which might be simple indicators of the form $g_u(A) = 1_{u \in A}$ and others could be cycle matroid rank functions in order to reduce any chance of the unachievability mentioned.
in Theorem 6.26). Even in cases where a DSF can be represented by an SCMM, DSFs may be a far more parsimonious representation of classes of submodular functions and hence a more efficient family over which to learn, analogous to results in DNNs showing the need for exponentially many hidden units for shallow networks to implement a network with more layers [40].

Suppose \( f \in C_n \) is a target submodular function, \( f_w \in \text{DSF}_k \) is a parameterized \( k \)-layer DSF, \( D = \{(S_i, y_i)\}_i \) is a training set consisting of subsets \( S_i \subseteq V \) and valuations \( y_i = f(S_i) \) for the target function and that is drawn from distribution \( \mathbf{Pr} \). An empirical risk minimization (ERM), or regression, style of learning is obtained a standard way:

\[
\min_{w \in W} J(w) = \sum_i L(y_i, f_w(S_i)) + \|w\| \quad (107)
\]

where \( L(\cdot, \cdot) \) is a loss function and \( \|w\| \) is a norm on the parameters. Obvious candidates for the loss would be squared loss, or L1 loss, and the norm can also be chosen to prefer smaller values for \( w \). Given the objective \( J(w) \) one may proceed using, for example, projected stochastic gradient descent, where at each step we project the weights \( w \) into \( W \) which corresponds to the non-negative orthant for parameters other than \( m_A \) to ensure submodularity is retained. Under this approach, and with an appropriate regularizer, it may be feasible to obtain generalization bounds in some form [135] as is often found in statistical machine learning settings. Note that, depending on the loss \( L \) used, this approach may be tolerant of noisy estimates of the function, where, say, \( y_i = f_w(S_i) + \epsilon \) and where \( \epsilon \) is noise, somewhat analogous to how it is possible to optimize a noisy submodular function [59]. Alternatively, one could analyze it under an agnostic learning setting.

Under many distribution assumptions, such as when \( \mathbf{Pr} \) is the uniform distribution over \( 2^V \), then as the training set gets larger, we approach the case where there are \( O(2^V) \) distinct samples, and the goal is to learn the function at all points. For large ground sets, certain learning settings might become infeasible in practice due to the curse of dimensionality. As mentioned above, there are learning settings that ask only for a fraction \( 1 - \beta \) of the points to be learnt, but without a mechanism to specify which fraction.

In many practical learning situations, however, access to an oracle function \( h(A) \), or training data that utilizes \( h \)'s evaluations, might not be available. Even if \( h \) available, such a learning setting might be overkill for certain applications, as we might not need a submodular function \( f_w \) to be accurate at all points \( A \subseteq V \). One example is in summarization applications [92, 150] where we wish to learn a submodular function \( f_w \) that, when maximized subject to a cardinality constraint, produces a set that is valued highly by the true submodular function relative to other sets of that size. Such a set should be diverse and high quality. In this case, one does not need \( f_w \) to be an accurate surrogate for \( f \) except on sets \( A \) for which \( f \) is large. More precisely, instead of trying to learn \( f \) everywhere, we seek only to learn the parameters \( w \) of a function so that if \( B \in \text{argmax}_{A \subseteq V : |A| \leq k} f_w(A) \), then \( h(B) \geq \alpha h(A^*) \) for some \( \alpha \in [0, 1] \) where \( A^* \in \text{argmax}_{A \subseteq V : |A| \leq k} h(A) \). This setting puts fewer constraints on what is needed to be learnt than the regression approach and hence should correspondingly be easier. This is somewhat analogous to discriminative learning where the entire distribution over input and output variables is not needed and instead only a conditional distribution (or a deterministic mapping from input to output) is required.

The max-margin approach [140, 92, 150] is appropriate to this problem and is applicable to learning DSFs. Given an unknown but desired non-negative submodular function \( f \in C_n \), we are given a set of representative sets \( S = \{S_1, S_2, \ldots \} \), with \( S_i \subseteq V \) and where each \( S \in S \) is scored highly by \( f(\cdot) \). Unlike the regression approach, we do not need the actual evaluations \( f(S_i) \). It might be, for example, that the sets are selected summaries chosen by a human annotator from a larger set. A matroid analogy is to learn a matroid using a set of independent sets of a particular size, say \( \ell \). If \( M' = (V, I') \) is a matroid of rank \( \ell' > \ell \), then \( M = (V, I) \) is also a matroid where \( I = \{I \in I' : |I| \leq \ell \} \).

In max-margin approach, we learn the parameters \( w \) of \( f_w \) in an attempt to make, for all \( S \in S \), \( f_w(S) \) high, while for \( A \in 2^V \), \( f_w(A) \) is lower by a given loss. More precisely, we ask that for \( S \in S \) and \( A \in 2^V \), \( f_w(S) \geq f_w(A) + \ell_S(A) \). The loss is chosen so that \( \ell_S(S) = 0 \), so that \( \ell_S(A) \) is very small whenever \( A \) is close to \( S \) (e.g., if \( A \) is also a good summary), and so that \( \ell_S(A) \) is large when \( A \) is considered much worse (e.g., if \( A \) is a poor summary). Achieving the above is done by maximizing the loss-dependent margin, and reduces to finding parameters so that \( f_w(S) \geq \max_{A \in 2^V} [f_w(A) + \ell_S(A)] \) is satisfied for \( S \in S \). The task of finding the maximizing set is known as loss-augmented inference (LAI) [146, 160], which for general \( \ell(A) \) is
NP-hard. With regularization, the optimization becomes:

$$\min_{w \in \mathcal{W}} \sum_{S \subseteq \mathcal{S}} \mathcal{L} \left( \max_{A \in 2^\mathcal{V}} [f_w(A) + \ell_S(A)] - f_w(S) \right) + \frac{\lambda}{2} ||w||^2_2.$$  \hspace{1cm} (108)

where $\mathcal{L}$ is a classification loss function such as the logistic ($\mathcal{L}(x) = \log(1 + \exp(-x))$) or hinge ($\mathcal{L}(x) = \max(0, x)$) loss. If it is the case that $f_w(S)$ is linear in $w$ (such as when $w$ are mixture parameters in an SCMM as was done in \cite{140, 92, 150}), and if the maximization can is done exactly, then this constitutes a convex minimization procedure. In general, however, there are several complications.

Firstly, the LAI problem $\max_{A \in 2^\mathcal{V}} [f_w(A) + \ell_S(A)]$ may be hard. Given a submodular function for the loss, as was done in \cite{92}, then the greedy algorithm offers the standard $1 - 1/e$ approximation guarantee for LAI. On the other hand, a submodular function is not always natural for the loss. Recall above that $\ell_S(A)$ should be large when $A$ is considered a poor set relative to $S$ (e.g. if $A$ is a poor summary). If it is the case that one may get an assessment of $A$, say via a surrogate $\tilde{f}$ of the ground truth function $f$, then one may use $\ell_S(A) = \kappa - \tilde{f}(A)$ but this, to the extent that $\tilde{f}$ needs to represent $f$, approaches the labeling needs of the ERM/regression approach above. If $\tilde{f}$ is submodular, then $\kappa - \tilde{f}$ is supermodular, and in this case solving $\max_{A \in 2^\mathcal{V} \setminus S} [f(A) + \ell(A)]$ involves maximizing the difference between two submodular functions, and the submodular-supermodular procedure \cite{110, 64} can be used although this procedure does not have guarantees in general.

Secondly, when $f_w$ is not linear in $w$, the above problem is not convex. Given the enormous success of deep neural networks in addressing non-convex optimization problems, however, this should not be daunting. Indeed, given an estimation to $\tilde{A} \in \arg\max_{A \in 2^\mathcal{V}} [f_w(A) + \ell_S(A)]$, we can easily obtain an approximate subgradient of weights $\partial_w (f_w(\tilde{A}) - f_w(S) + \lambda/2 ||w||^2_2)$ to be used in a projected stochastic subgradient descent procedure. For a DSF, this subgradient can be easily computed using backpropagation, similar to the approach of \cite{121}. Like in the mixtures case, we must use projected descent to ensure $w \in \mathcal{W}$ and submodularity is preserved. Recall, however, that the weights corresponding to $m_{\pm}(A)$ may be left negative if they so choose. Preliminary experiments in learning DSFs in this fashion were reported in \cite{37} and show encouraging results.

As an additional benefit, many of the concave functions mentioned in Section 3.1 are parameterized themselves, and these parameters may also be the target of stochastic gradient based learning. In such case, not only the weights but also the concave functions of a DSF may be learnt.

Given the ongoing research on the non-convex learning of DNNs, which have achieved remarkable results on a plethora of machine learning tasks \cite{87, 54}, and given the similarity between DSFs and DNNs, we may leverage the same DNN learning techniques to learn DSFs. This includes stochastic gradient descent, convolutional linear maps, momentum, dropout, batch normalization, unsupervised pre-training, learning rate scheduling such as AdaGrad/Adam, convolutional matrix patterns, mini-batching, and so on. In some cases these methods might need to be modified (e.g., stochastic projected gradient descent to ensure the function remains submodular). Moreover, the suitability of fast GPU computing to the matrix-matrix multiplications necessary to evaluate DSFs should also be a benefit. Lastly, the many toolkits that support DNN training (such as Tensorflow, Theano, Torch, Caffe, CNTK, and so on), and that include automatic symbolic differentiation and semi-differentiation (for non-differentiable functions) for backpropagation-style parameter learning can easily be used to train DSF. All of these techniques and software may be leveraged to DSF’s benefit, and is true both for the regression and max-margin setting.

### 7.1.1 Training and Testing on Different Ground Sets, and Multimodal Submodularity

In the training process in machine learning, one trains with a training set and then evaluates or tests on a distinct set having no overlap with the training set. When training submodular functions, this means that the training set might consist of multiple ground sets, and the test set might consist of ground sets that were not seen during training. A data set might consist of $\mathcal{D} = \{(V_i, S_i, y_i)\}_i$ where $V_i$ is a ground set, $S_i \subseteq V_i$ and, when available, $y_i = f_i(S_i)$ is an evaluation of $S_i$ by a ground-set-specific submodular function $f_i$. Hence, there may be no instance where two ground sets are the same, so $V_i \neq V_j$ for $i \neq j$, nor might there be ground set commonality between training and test data sets. The reason this occurs can be explained using a document summarization example \cite{92}. A training set consists of pairs, each of which is pile of documents (comprised of a set of sentences) and a subset of those sentences corresponding to a summary.
Multiple training samples consists of different piles of documents and their corresponding summaries, and then a test set consists of a different pile of documents and summaries thereof. In this section, we discuss how to addresses this problem for DSFs via a strategy that generalizes [92, 150].

Let $V$ be a training set where each $v \in V$ is a data object. Any particular element $v \in V$ may be represented by a vector of non-negative weights $(w^{(0)}_1(v), w^{(0)}_2(v), \ldots, w^{(0)}_{|U|}(v))$. Each object $v \in V$ is hence embedded in non-negative $|U|$-dimensional space corresponding to low-level features $U$ for the object. For example, if $v$ is a sentence, $w^{(0)}_u(v)$ might counts the number of times an n-gram $u$ appears in sentence $v$. Alternatively, $w^{(0)}_u(v)$ might be automatically obtained via representation learning in a DNN-based auto-encoder, or there can be a mix of features obtained via representation learning and hand-crafting, using any of the feature-engineering methods discussed in Section 3.1. For each feature, we can define a modular function $m_u(A) = \sum_{a \in A} w^{(0)}_u(a)$ that measures feature $u$’s weight for any set $A \subseteq V$. The entire training set, therefore can be seen a matrix $w^{(0)}$ to be used as the first layer in DSF (e.g., $w^{(0)}$ in Figure 6 left (red)) that is fixed during the training of subsequent layers (Figure 6 left (green)). As long as $w^{(0)}$ is non-negative, submodularity is preserved and if $w^{(0)}$ is constant, it allows all later layers (i.e., $w^{(2)}, w^{(3)}, \ldots$) to be learnt generically over any heterogenous set of objects that can be represented in the same feature space, including multimodal data objects (e.g., consisting of images, videos, and text sentences). Any training process remains ignorant that this is happening since it sees the data only post feature representation. In fact, one can view this, in light of Theorem 5.12, as a fixed layer consisting of an SCMM that embeds data objects into feature space corresponding to the components of the SCMM.

Once training has occurred, and if there is an analogous process to transform distinct (and possibly different types) of test data into the same feature space, it is possible to use the learnt DSF even for a different ground set. In Figure 6 right (red), we have a different transformation $w'^{(0)}$ into the same feature space $V^{(1)}$ which can use the DSF (green) learnt during training. This process analogous to the “shells” of [92]. In that case, mixtures were learnt over fixed components, some of which were graph based (and hence required $O(n^2)$ calculation for element-pair similarity scores). Via featurization in the first layer of a DSF, however, we may learn a DSF over a training set, preserving submodularity, avoid any $O(n^2)$ cost, and test on any new data represented in the same feature space. Alternatively, one could combine the shells approach and $w'^{(0)}$ into a vector of polymatroid functions and then apply Theorem 5.12.

### 7.2 Deep Supermodular Functions and Deep Differences

All of the results in this paper assume that the hidden units in a DSF are concave. If we replace these concave functions in Equation (11) then we get a class we could call Deep Supermodular Functions (DSUFs). The results in this paper, hence, generalize to show that DSUFs correspond to a larger class than just sums of convex functions composed with non-negative modular functions.
In [110, 64] it was shown that any set function \( h : 2^V \rightarrow \mathbb{R} \) can be represented as a difference between two submodular functions. If we take \( f_1, f_2 \in \text{DSF} \) then the class of functions \( \text{DDSF} = \{ h : h = f_1 - f_2, f_1, f_2 \in \text{DSF} \} \) can be seen as a class of deep differences of submodular functions. Considering the class \( \text{DSUF} = \{ h : h = f + g, f \in \text{DSF}, g \in \text{DSUF} \} \) can be seen as a class of deep submodular plus supermodular functions. Given that DSFs do not comprise all submodular functions, it is unlikely that DSUFs comprise all set functions. However, these can be useful classes of functions to learn over using, say, the deep learning methods mentioned in Sections 7.1. A key advantage of learning over this family is that the framework never looses the decomposition into two submodular functions or a submodular and supermodular function. For example, after learning, we can utilize submodular level-set constrained submodular optimization of the kind developed in [66] for optimization. Learning under such a decomposition, moreover, might reveal substitutive (via \( f \)) and complementary (via \( g \)) properties of the data.

It may also be useful to define a class of deep “cooperative-competitive” energy functions for use in a probabilistic model. For example, one can define probability distributions \( p \) over binary vectors with \( p(x) = \frac{1}{Z} \exp(f_w(x) - f_{w_2}(x)) \) where \( f_w \) and \( f_{w_2} \) are both deep submodular, or \( p(x) = \frac{1}{Z} \exp(f_w(x) + g_{w_2}(x)) \) where \( f_w \) is deep submodular and \( g_{w_2} \) is deep supermodular. If \( f_w \) and \( g_{w_2} \) have decomposition properties with respect to a graph, then these could be called deep cooperative-competitive graphical models.

### 7.3 Deep Multivariate Submodular Functions

Submodular functions have been generalized in a variety of ways to domains other than just subsets of a finite set \( V \) (i.e., binary vectors). In Section 5.2, we discussed the negativity of the off-diagonal Hessian as a way of defining submodular functions on lattices. Other ways to generalize submodularity considers discrete generalizations of properties such as midpoint convexity over integer lattices [109].

In this section, we consider certain submodular generalizations to multi-argument functions. For example, a set function \( f(A, B) \) with two arguments \( A \subseteq V \) and \( B \subseteq V \) is a biset function. If the domain is of the form \( 2^V \triangleq \{ (A, B) : A \subseteq V, B \subseteq V \} \), we may define the class of functions known as simple bisubmodular:

**Definition 7.1 (Simple Bisubmodularity [139])**. \( f : 2^V \rightarrow \mathbb{R} \) is simple bisubmodular iff for each \( (A, B) \in 2^V \), \((A', B') \in 2^V\) with \( A \subseteq A', B \subseteq B' \) we have for \( s \notin A' \) and \( s \notin B' \):

\[
\begin{align*}
    f(A + s, B) - f(A, B) &\geq f(A' + s, B') - f(A', B'), \\
    f(A, B + s) - f(A, B) &\geq f(A', B' + s) - f(A', B').
\end{align*}
\]

An equivalent way to define simple bisubmodularity is as follows.

**Proposition 7.2**. The function \( f : 2^V \rightarrow \mathbb{R} \) is simple bisubmodular whenever \( \forall (A, B), (A', B') \in 2^V \),

\[
f(A, B) + f(A', B') \geq f(A \cup A', B \cup B') + f(A \cap A', B \cap B') \quad (109)
\]

If the domain is of the form \( 3^V \triangleq \{ (A, B) : A \subseteq V, B \subseteq V, A \cap B = \emptyset \} \), then we can define directed bisubmodularity as follows:

**Definition 7.3 (Directed Bisubmodularity [125])**. Biset function \( f : 3^V \rightarrow \mathbb{R} \) is directed bisubmodular whenever

\[
f(A, B) + f(A', B') \geq f(A \cap A', B \cap B') + f((A \cup A') \setminus (B \cup B'), (B \cup B') \setminus (A \cup A')). \quad (110)
\]

Directed bisubmodularity functions have been generalized to what is known as \( k \)-submodular functions in [80, 62]. More recently, simple bisubmodularity [139] has been generalized to multivariate submodular functions [134]. A multivariate submodular (or what we will call a \( k \)-multi-submodular) function \( f : (2^V)^k \rightarrow \mathbb{R} \) is defined as a function such that for all \( (X_1, X_2, \ldots, X_k), (Y_1, Y_2, \ldots, Y_k) \in (2^V)^k \), we have that:

\[
f(X_1, X_2, \ldots, X_k) + f(Y_1, Y_2, \ldots, Y_k) \geq f(X_1 \cup Y_1, X_2 \cup X_2, \ldots, X_k \cup Y_k) + f(X_1 \cap Y_1, X_2 \cap X_2, \ldots, X_k \cap Y_k) \quad (111)
\]

These are not the same as \( k \)-submodular functions [62] but for \( k = 1 \) we obtain standard submodular functions and for \( k = 2 \) we obtain simple bisubmodular functions.
A DSF with \( k' > k \) layers can be used to instantiate a \( k \)-multi-submodular function. Consider a layered-DSF with \( k' \) layers corresponding to sets \( V^{(0)}, V^{(1)}, \ldots, V^{(k')} \). Choose a size \( k \) subset of these layers, say \( \sigma_1, \sigma_2, \ldots, \sigma_k \) where \( \sigma_j \in [0, k' - 1] \) for all \( j \), \( \sigma_1 = 0 \), and all of the \( \sigma_j \)'s are distinct, w.l.o.g., \( 0 = \sigma_1 < \sigma_2 < \cdots < \sigma_k \leq k' - 1 \). Given an \( f \in \text{DSF}_{k'} \), we ordinarily obtain a valuation \( f(A) \) using a subset \( A \subseteq V^{(0)} \) of the ground set. Now, consider \( f : (2^V)^k \rightarrow \mathbb{R} \) where \( A_1 \subseteq V^{(\sigma_1)}, A_2 \subseteq V^{(\sigma_2)}, \ldots, A_k \subseteq V^{(\sigma_k)} \) and the value of \( f(A_1, A_2, \ldots, A_k) \) is obtained as:

\[
\phi_{k'} \left( \sum_{v \in V^{(k')}} \sum_{v' \in V^{(k'-1)}} w_{v,v'}^{(k')} \phi_{v'v} \left( \sum_{v'' \in V^{(k-1)}} w_{v'',v'}^{(k-1)} \phi_{v''v'} \left( \sum_{v''' \in V^{(k-2)}} w_{v''',v''}^{(k-2)} \phi_{v''',v''} \left( \cdots \right) \right) \right) \right) + m_{1}(A_1) + m_{2}(A_2) + \cdots + m_{k}(A_k)
\]

where \( V^{(i)} = V^{(i)} \cap A_{\sigma_i}^{-1} \) whenever \( \forall j \in [0, k' - 1] : i = \sigma_j \) and otherwise \( V^{(i)} = V^{(i)} \), and where \( m_{j}(A_j) : V^{(\sigma_j)} \rightarrow \mathbb{R} \), for each \( j \), is an arbitrary modular function. In other words, \( A_j \) acts as a set of binary triggers to activate a set of units at layer \( j \) in the DSF. If we hold all but layer \( j \) fixed, then \( A_j \) can be seen as the set of units to provide the values for the vector \( b_{A_j} \), in Corollary 5.12.1 and as a result, we get as a result that the function is submodular in \( A_j \). \( k \)-multi-submodularly then follows from a generalization of Proposition 7.2 to \( k \)-multi-submodularity.

Deep \( k \)-multi-submodular functions should be useful in a number of applications, for example representing information jointly in a set of features and data items (and could be useful for simultaneous feature/data subset selection).

### 7.4 Simultaneously Learning Hash and Submodular Functions

One of the difficulties in training DSFs is obtaining a sufficient amount of training data. It would be useful therefore to have an strategy to easily and cheaply obtain as much training data as desired. In the spirit of the empirical success of DNNs, this section suggests one strategy for doing this.

The goal is to learn a map from a vector \( x \in \mathbb{R}^d \) to a \( b \)-bit vector via a function \( h_\theta : \mathbb{R}^d \rightarrow \{0, 1\}^b \), anywhere \( h_\theta \) is parameterized by \( \theta \). The reason for doing this is to pass data objects (e.g., images, documents, music files, etc.) that are represented in the input space and map them to binary space \( \{-1, 1\}^b \) where \( b < d \) and, moreover, since the space is binary, operations such nearest neighbor search are faster. There are existing approaches that can learn this mapping automatically, sometimes using neural networks (e.g., [56]). Often, \( h_\theta : \mathbb{R}^d \rightarrow \{-1, 1\}^b \) rather than \( h_\theta : \mathbb{R}^d \rightarrow \{0, 1\}^b \), but this should not be of any consequence.

This section describes a strategy for learning hash functions that utilizes DSFs, the Lovász extension, and the submodular Hamming metric [50]. Let \( f : 2^V \rightarrow \mathbb{R} \) be a submodular function and let \( f \) be its Lovász extension. Also, let \( d_f(A, B) = f(A \triangle B) \) be the submodular Hamming metric between \( A \) and \( B \) parameterized by submodular function \( f \). We are given a large (and possibly unlabeled) data set \( D = \{x_i\}_{i \in D} \) and a corresponding distance function between data pairs \( (d(x_i, x_j)) \) is the distance between item \( x_i \in \mathbb{R}^d \) and \( x_j \in \mathbb{R}^d \). The goal is to produce a mapping \( h_\theta : \mathbb{R}^d \rightarrow \{0, 1\}^b \) so that distances in the ambient space \( d(x_i, x_j) \) are preserved in the binary space. One approach adjusts \( h_\theta \) to ensure that \( d(x_i, x_j) = \sum_{t=1}^{b} 1_{b_{A}(x_i)(t) \neq b_{A}(x_j)(t)} \). That is, we adjust \( h_\theta(x_i) \) so that the Hamming distance preserves the distances in the ambient space.

In general, this problem is made more difficult by the rigidity of the Hamming distance. In order to relax this constraint, we can use a submodular Hamming metric parameterized by a DSF \( f_w \) (which itself is parameterized by \( w \)). Hence, the hashing problem can be seen as finding \( \theta \) and \( w \) so that the following is true as much as possible.

\[
d(x_i, x_j) = d_{f_w}(h_\theta(x_i), h_\theta(x_j))
\]

The function \( h_\theta \) maps to binary vectors, and \( d_{f_w} \) is a function on two sets. This makes it difficult to pass derivatives through these functions in a back-propagation style learning algorithm. To address this issue, we can further relax this problem in the following way:

- **Given** \( A, B \subseteq V \), the Hamming distance is \(|A \triangle B|\) and we can represent this as \((1_A \otimes (1_V - 1_B)) + (1_B \otimes (1_V - 1_A))(V)\) where \( \otimes : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^n \) is the vector element multiplication operator (i.e.,
[x \otimes y](j) = x(j)y(j)). In other words, we define a vector \(z_{A \triangle B} \in \{0, 1\}^V\) with

\[
z_{A \triangle B} = 1_A \otimes (1_V - 1_B) + 1_B \otimes (1_V - 1_A)
\]

(115)

and \(|A \triangle B| = z_{A \triangle B}(V) = \sum_{i \in V} z_{A \triangle B}(i)\). Hence, the submodular hamming metric is \(f(A \triangle B) = \bar{f}(z_{A \triangle B})\), which holds since the Lovász extension is tight at the vertices of the hypercube.

- For two arbitrary vectors \(z_1, z_2 \in [0, 1]^V\), we can define a relaxed form of metric as follows: \(d(z_1, z_2) = \bar{f}(z_1 + z_2 - 2z_1 \otimes z_2)\), and for a DSF, this can be expressed as \(d_{f_w}(z_1, z_2) = f_w(z_1 + z_2 - 2z_1 \otimes z_2)\).

- Let us suppose that \(\hat{h}_\theta : \mathbb{R}^d \rightarrow [0, 1]^b\) is a mapping from real vectors to vectors in the hypercube (e.g., \(\hat{h}_\theta\) might be expressed with a deep model with a final layer of \(b\) sigmoid units at the output to ensure that each output is between zero and one). Then we can construct a distortion between \(x_i\) and \(x_j\) via

\[
d_{w, \theta}(x_i, x_j) \triangleq d_{f_w}(\hat{h}_\theta(x_i), \hat{h}_\theta(x_j)) = f_w(\hat{h}_\theta(x_i) + \hat{h}_\theta(x_j) - 2\hat{h}_\theta(x_i) \otimes \hat{h}_\theta(x_j))
\]

(117)

Hence, \(d_{w, \theta}\) is a parametric family of distortion functions that uses two maps, one via the DNN \(\hat{h}_\theta\) and another via the DSF \(f_w\) using the Lovasz extension \(\bar{f}\).

- Assuming the original unlabeled data set \(\mathcal{D}\) is large, and the distance function in the ambient space is accurate, it may be possible to learn both \(w\) and \(\theta\) by forming an objective function to minimize:

\[
J(w, \theta) = \sum_{i,j \in \mathcal{D}} \|d(x_i, x_j) - d_{w, \theta}(x_i, x_j)\|.
\]

(118)

Learning (\(\min_{w, \theta} J(w, \theta)\)) can utilize stochastic gradient steps and the entire arsenal of DNN training methods.

The approach learns both the mapping function \(\hat{h}_\theta\) and the submodular function \(f_w\) simultaneously in a way that preserves the original distances. It may therefore be that \(\hat{h}_\theta\) can be used as a feature transformation (i.e. a way to map data objects \(x\) into feature space via \(\hat{h}_\theta\)), and at the same time we obtain a submodular function \(f_w\) over those features that, perhaps, can useful for summarization, all without needing labeled training data as in Section 7.1.

8 Conclusions and Future Work

In this paper, we have provided a full characterization of our newly-proposed class of submodular functions, DSFs. We have introduced the antitone gradient as a way of establishing subclasses of submodular functions. We have shown that DSFs constitute a strictly larger family than the family of submodular functions obtained by additively combining concave composed with modular functions (SCMMs). We have also shown that DSFs do not comprise all submodular functions. This was all done in the special context of matroid rank functions, and also in a more general context.

As mentioned at various points within the paper, there are several interesting open problems associated with DSFs. An immediate task is to further develop practical strategies for successfully empirically learning DSFs, as was initiated in [36]. A second task is to establish generalization bounds for learning DSFs in an ERM framework. A third task asks if there is a finite set of “boot” submodular functions that, when cascaded into a DSF as in Theorem 5.12, lead to a family that comprises all polymatroid functions. And lastly, it remains to compare the DSF family with the family of all entropy functions [163].

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A More General Conditions on Two-Layer Functions: Proofs

Proof of Theorem 6.5. We begin with the “only if” part. In the proof, we always assume the ground set $V = \{a, b, c, d, e, f\}$.

**Definition A.1.** Consider the bijection $p : V \rightarrow V$. Let $A_p = \{p(v) | v \in A\}$. Notationally, we may write a given $p$ as $(v_1, v_2, \ldots, v_k) \rightarrow (u_1, u_2, \ldots, u_k)$ where $u_i, v_i \in V$ with $u_i = p(v_i)$. Let $P_A$ be the set of all one-to-one maps that are an identity for $v \in V \setminus A$, that is $p(v) = v$ for all $v \in V \setminus A$. Corresponding to Theorem 6.5, in the below, assume $V = \{a, b, c, d, e, f\}$. We next define a number of operators that allow us to study the partial permutation symmetry of a set function.

**Definition A.2.** For any submodular function $h$, let:

- $E_B$ be an operator such that $E_B h(A) = \frac{1}{|P_A|} \sum_{p \in P_A} h(A_p)$;
- $E'$ be an operator such that $E' h(A) = \frac{1}{2} [h(A) + h(A_{(a,b,c,d,e,f) \rightarrow (d,e,f,a,b,c)})]$.
Lemma A.3. \( Eg(A) = g(A) \) for all \( A \subseteq V \). Also, \( E \) is a linear operation, that is \( E(h_1 + h_2) = Eh_1 + Eh_2 \). Lastly, if \( h \) is an SCMM, \( Eh \) is also an SCMM.

Lemma A.4. For any \( A, B \subseteq V \), if \(|A \cap \{a, b, c\}| = |B \cap \{a, b, c\}| \) \( \land \) \(|A \cap \{d, e, f\}| = |B \cap \{d, e, f\}| \) \( \lor \) \(|A \cap \{a, b, c\}| = |B \cap \{d, e, f\}| \) \( \land \) \(|A \cap \{d, e, f\}| = |B \cap \{a, b, c\}| \), then \( Eh(A) = Eh(B) \).

This means that \( Eh(A) \) is fully determined by the unordered pair \(|A \cap \{a, b, c\}|, |A \cap \{d, e, f\}|\).

Definition A.5. For any \( h : 2^V \rightarrow \mathbb{R}, \) define \( Eh(n_1, n_2) = Eh(A) \), where \( n_1 = |A \cap \{a, b, c\}|, n_2 = |A \cap \{d, e, f\}| \), and \( 0 \leq n_2 \leq n_1 \leq 3 \).

Since this section shows the “only if” part of Theorem 6.5, we have \( g(A) \) is an SCMM, thus by Lemma 5.9, \( g(A) = \sum_i \min(m_i(A), \beta_i) + m_{\pm}(A) \), where \( m_i \geq 0 \) is non-negative modular and \( \beta_i > 0 \). Immediately, we have

\[
Eg(A) = \sum_i E \min(m_i(A), \beta_i) + Em_{\pm}(A) \tag{119}
\]

\[
g(A) = \sum_i Eg_i(A) + Em_{\pm}(A) \tag{120}
\]

according to lemma A.3, where \( g_i(A) = \min(m_i(A), \beta_i) \). Moreover, we assume \( m_i(V) > \beta_i > 0 \) for each \( i \); otherwise \( g_i \) is modular and can be merged into the final modular term. Furthermore, we assume that \( m_i(v) \leq \beta_i \) for all \( v \in V \) and all \( i \). If \( m_i(v) > \beta_i \), then \( \min(m_i(A), \beta_i) = \beta_i \) whenever \( v \) is selected in \( A \). In such case, we can let \( m_i(v) = \beta_i \) which have the same function value for all \( A \). Therefore we have

Lemma A.6. \( g_i(V \setminus \{v\}) < g_i(v) = m_i(v) \) for all \( i \) and \( v \) s.t. \( m_i(v) > 0 \). In other words, \( I_{g_i}(V \setminus \{v\}) > 0 \) for all \( i \) with \( g_i(v) > 0 \).

Proof. This follows since \( m_i(V) \) passes the linear part of \( g_i \) but \( m_i(v) \) does not.

Lemma A.7. \( g_i(a \{b, c\}) = g_i(a \{b, c, d, e, f\}) \) for all \( i \).

Proof. We have that \( 0 \leq I_g(a; A) \leq I_g(a; B) \) for all \( A \subseteq B \). Hence \( I_g(a; \{b, c, d, e, f\}) = 0 \) implies \( I_g(a; \{b, c\}) = 0 \). Hence, for all \( i \), \( I_{g_i}(a; \{b, c, d, e, f\}) = I_{g_i}(a; \{b, c\}) = 0 \), implying \( g_i(a \{b, c\}) = g_i(a \{b, c, d, e, f\}) \) for all \( i \).

Definition A.8. We define the following functions:

- \( f_0(A) = |A| \);
- \( f_1(A) = \min(|A \cap \{a, b, c, d, e, f\}|, 1) \);
- \( f_2(A) = \min(|A \cap \{a, b, c, d, e, f\}|, 2) \);
- \( f_3(A) = \min(|A \cap \{a, b, c\}|, 1) + \min(|A \cap \{d, e, f\}|, 1) \);
- \( f_4(A) = \min(|A \cap \{a, b, c\}|, 2) + \min(|A \cap \{d, e, f\}|, 2) \);
- and \( f_5(A) = E \min((1, 1, 0, 0.5, 0.5, 0.5)^T(A), 1) \) where \((x_a, x_b, x_c, x_d, x_e, x_f)^T\) is a modular function with elements \( x_a, x_b, x_c, x_d, x_e, x_f \).

Immediately, we notice that \( Ef_i = f_i \) for all \( i \).

Lemma A.9. For a normalized monotonically non-decreasing submodular \( h \), if \( h(\{d, e, f\}) = 0 \), then \( Eh \) is a conical combination of \( f_0, f_3, f_4 \).

Proof. Let \( x = \frac{1}{3}(h(a) + h(b) + h(c)) \) and \( y = \frac{1}{2}(h(\{a, b\}) + h(\{b, c\}) + h(\{a, c\})) \) and \( z = h(\{a, b, c\}) \). Then \( Eh \) can actually be written as \( \frac{1}{3}[(z - y)f_0 + (2x - y)f_3 + (2y - z - x)f_4] \) where \( z - y, 2x - y, 2y - z - x \geq 0 \) according to submodularity.
Lemma A.10. We say a function is fully curved if \( f(v|V \setminus v) \) for some \( v \). For \( i \) such that \( g_i \) is not fully curved, \( E g_i \) is a conical combination of \( f_0, f_3, f_4 \).

Proof. Without lose of generality, we assume \( g_i(a|\{b, c, d, e, f\}) > 0 \). Immediately we have \( m_i(a) > 0 \) and \( m_i(\{b, c, d, e, f\}) < \beta_i \). According to lemma A.6 and lemma A.7, we have \( I(a; \{b, c\}) = g_i(a) - g_i(a|\{b, c\}) = g_i(a) - g_i(\{a\}|\{b, c\}) > 0 \). Thus \( m_i(\{a, b, c\}) \geq \beta_i \). Therefore \( 0 = g_i(a|\{b, c\}) - g_i(\{b, c\}) = g_i(\{a, b, c\}) - g_i(\{a, b, c, d, e, f\}) + g_i(\{b, c, d, e, f\}) = \beta_i - m_i(\{b, c\}) - m_i(\{b, c, d, e, f\}) = m_i(\{d, e, f\}) \). So we have that \( m_i(\{d, e, f\}) = 0 \) and \( g_i \) only involves \( a, b, c \). According to lemma A.9, \( E g_i \) is a conical combination of \( f_0, f_3, f_4 \).

Lemma A.11. \( m \pm \) is not necessary, that is if we find one SCMM expansion of \( g \), we can also find another SCMM expansion with \( m \pm = 0 \).

Proof. For some \( i \), \( E g_i \) is fully curved and for the other \( i \), \( E g_i = g'_i + m'_i \) where \( g'_i \) is a fully curved SCMM and \( m'_i \) is modular according to lemma A.10. So we can group all \( m'_i \) and \( m \pm \) together. If a fully curved submodular function is another fully curved submodular function plus modular, the only possibility is that the modular term equals 0. So the final modular vanishes.

So actually, we can ignore the final modular functions at the expansion of \( g \). \( g(A) = \sum_i \min(m_i(A), \beta_i) = \sum_i E g_i(A) \), where all term are non-negative and fully curved now.

Consider the quality \( g_i(a|\{b, c\}) \), it is non-negative for each \( i \) and 0 for \( g \). So for each \( i \), we have \( g_i(\{a|\{b, c\}) = 0 \). In fact, \( g_i \) is fully curved on \( \{a, b, c\} \) and \( \{d, e, f\} \).

Lemma A.12. For a normalized monotonically non-decreasing submodular \( h \), if \( h \) is fully curved on \( \{a, b, c\} \) and \( \{d, e, f\} \), then \( E h \) is determined by 5 values, \( E h(1, 0), E h(2, 0), E h(1, 1), E h(2, 1) \) and \( E h(2, 2) \).

Proof. According to lemma A.4 and definition A.5, \( E h(A) \) is determined by \( E h(1, 0), E h(1, 1), E h(2, 0), E h(2, 1), E h(2, 2), E h(3, 2) \) and \( E h(3, 3) \). But \( E h(n_1, n_2) = E h(\min(n_1, 2), \min(n_2, 2)) \) according to the saturate properties. So \( E h(1, 0), E h(2, 0), E h(1, 1), E h(2, 1) \) and \( E h(2, 2) \) are the only free variables remained.

Lemma A.13. \( E h(n_1, n_2) = E h_1(n_1, n_2) + E h_2(n_1, n_2) \) if \( h = h_1 + h_2 \).

So in fact \( E f \) is a 5-dimensional-vector. Here we calculate the 5-dimensional-vector for \( f_1, f_2, f_3, f_4, f_5 \), see table 1.

Table 1: Function values

| \( E f(1, 0) \) | \( E f(2, 0) \) | \( E f(1, 1) \) | \( E f(2, 1) \) | \( E f(2, 2) \) |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| \( f_1 \)       | 1               | 1               | 1               | 1               |
| \( f_2 \)       | 1               | 2               | 1               | 2               | 2               |
| \( f_3 \)       | 1               | 1               | 2               | 1               | 2               |
| \( f_4 \)       | 1               | 2               | 2               | 3               | 4               |
| \( f_5 \)       | \( \frac{1}{2} \) | 1               | \( \frac{3}{2} \) | 1               | 1               |

Lemma A.14. For all \( i \), \( E g_i \) is a conical combination of \( f_1, f_2, f_3, f_4, f_5 \).

Proof. For \( i \) s.t. \( g_i(\{a, b, c\}) = 0 \) or \( g_i(\{d, e, f\}) = 0 \), \( E g_i \) is a conical combination of \( f_0, f_3, f_4 \) according to lemma A.9. Moreover, \( f_0 \) is not necessary since \( g_i \) is fully curved.

For other \( i \), if \( m_i(a) + m_i(b) < \beta_i \), then \( m_i(c) = 0 \); otherwise \( g_i(c|\{a, b\}) = 0 \). But in this case \( 0 = g_i(a|\{b, c\}) = m_i(a) \) and \( 0 = g_i(b|\{a, c\}) = m_i(b) \) which contradicts with \( g_i(\{a, b, c\}) > 0 \). So \( m_i(\{a, b\}) \geq \beta_i \). Similarly, we have \( m_i(\{b, c\}), m_i(\{c, a\}), m_i(\{d, e\}), m_i(\{e, f\}), m_i(\{d, f\}) \geq \beta_i \).

So \( E g_i(2, 0) = E g_i(2, 1) = E g_i(2, 2) = \beta_i \). And the undecided parameters are \( E g_i(1, 0) \) and \( E g_i(\{1, 1\}) \).

It is easy to check that \( E g_i = |E g_i(1, 1) + 2E g_i(1, 0) - 2\beta_i|f_1 + \frac{1}{2}|5E g_i(1, 1) - 2E g_i(1, 0) - 3\beta_i|f_2 + |6\beta_i - 6E g_i(1, 1)||f_5 \).
Lemma A.15. Given \( g_i(A) = \min(m_i(A), \beta_i) \), if \( m_i(a) + m_i(b) + m_i(c) + m_i(d) + m_i(e) + m_i(f) \geq \beta_i \), we have \( E_g(1,1) + 2E_g(1,0) - 2\beta_i \geq 0 \), so \( E_g(1,1) - 2E_g(1,0) - 3\beta_i \geq 0 \), \( E_g(1,1) \leq \beta_i \).

Proof. Let \( x_i \) be the weight of each elements. Without lose of generality, we assume that \( \beta_i \geq x_1 \geq x_2 \geq x_c \geq 0 \), \( \beta_i \geq x_d \geq x_e \geq x_f \geq 0 \) and \( x_c \geq x_f \).

\[ E_g(1,0) = \frac{1}{2} \sum_i x_i \geq \frac{3}{2} \beta_i \text{ and } E_g(1,1) = \frac{1}{2} \sum v \in \{a,b,c\} \sum u \in \{d,e,f\} g_i(\{v,u\}) = \frac{5}{4} \beta_i + \frac{1}{4} \min(x_a + x_f, \beta_i) + \min(x_b + x_f, \beta_i) + \min(x_c + x_f, \beta_i) \geq \frac{3}{2} \beta_i. \]

Therefore, \( E_g(1,1) + 2E_g(1,0) - 2\beta_i \geq 0 \) and \( E_g(1,1) \leq \beta_i \).

For \( 5E_g(1,1) - 2E_g(1,0) - 3\beta_i \geq 0 \), if \( x_c + x_f \geq \beta_i \), we have \( E_g(1,1) = \beta_i \) and \( E_g(1,0) \leq \beta_i \). So \( 5E_g(1,1) - 2E_g(1,0) - 3\beta_i \geq 0 \).

If \( x_c + x_f \leq \beta_i \), 5 \( E_g(1,1) + 2E_g(1,0) - 3\beta_i \) is growing when \( x_f \) increased. So we can let \( x_f = 0 \) for the worst case. Therefore \( 5E_g(1,1) + 2E_g(1,0) - 2\beta_i = 5(\frac{5}{4} \beta_i + \frac{1}{4} [x_a + x_b + x_c]) - \frac{1}{4} [x_a + x_b + x_c + x_d + x_e] - 3\beta_i \) which is increasing with respect to \( x_a, x_b, x_c \) and deceasing with respect to \( x_d, x_e \). Further more, we have \( \frac{5}{4} \beta_i \leq x_a + x_b + x_c \) and \( x_d + x_e \leq 2\beta_i \). So \( 5E_g(1,1) + 2E_g(1,0) - 2\beta_i \geq 0 \)

Therefore, we have shown that \( E_g \) is a conical combination of \( f_1, f_2, f_3, f_4, f_5 \) for all \( i \). Therefore \( g = \sum_i E_g_i \) is a conical combination of \( f_1, f_2, f_3, f_4, f_5 \).

The 5-vector related to \( E_g \) is \((\phi(1), \phi(2), \phi(2), \phi(3), \phi(4))\). So according to Table 1, the unique expression to expand \( g \) on \( f_1, f_2, f_3, f_4 \) is \( g(A) = [2\phi(1) + \phi(2) - 4\phi(3) + 2\phi(4)]f_1 + [-\phi(1) + 3.5\phi(2) - 4\phi(3) + 1.5\phi(4)]f_2 + [-\phi(2) + 2\phi(3) - \phi(4)]f_3 + [-\phi(3) + \phi(4)]f_4 + [-\phi(3) - \phi(4)]f_5 \)

This expression is valid if and only if \( -\phi(1) + 3.5\phi(2) - 4\phi(3) + 1.5\phi(4) \geq 0 \) and \( 2\phi(1) + \phi(2) - 4\phi(3) + 2\phi(4) \geq 0 \); other coefficients are always non-negative according to concavity and monotonicity.

The “if” part is straightforward according to the above expansion as we saw after the statement of the theorem.

B Sums of Weighted Cardinality Truncations is Smaller than SCMMs

In this section, show Lemma 5.10, namely that \( G = \{ \sum_{B \subseteq V} \sum_{i=1}^{\left| B \right| - 1} \alpha_{B,i} \min(|A \cap B|, i), \forall B, i, \alpha_{B,i} \geq 0 \} \subset \text{SCMM} \). We assume the reader is familiar with the notation in Appendix A.

Lemma B.1. \( f_5(A) \notin \{ \sum_{B \subseteq V} \sum_{i=1}^{\left| B \right| - 1} \alpha_{B,i} \min(|A \cap B|, i) | \alpha_{B,i} \geq 0 \} \)

Proof. Assume that

\[ f_5(A) = \sum_{B \subseteq V} \sum_{i=1}^{\left| B \right| - 1} \alpha_{B,i} \min(|A \cap B|, i) = \sum_{B \subseteq V} \sum_{i=1}^{\left| B \right| - 1} \alpha_{B,i} E \min(|A \cap B|, i). \]  

(121)

Note that \( f_5 \) is fully curved on \( \{a,b,c\} \) and \( \{d,e,f\} \), and these hold for all terms. So for \( B \) and \( i \), if \( i \geq |B \cap \{a,b,c\}| \) or \( i \geq |B \cap \{d,e,f\}|, \alpha_{B,i} = 0 \). Therefore the remaining terms are \( f_1, f_2, f_3, f_4, E \min(|A \cap \{a,b,d,e\}|, 1) \) and \( E \min(|A \cap \{a,b,c,d,e\}|, 1) \). Therefore, for all these functions, \( E\{2,0 \} \leq \frac{9}{8} E\{1,1 \} \), but \( E\{2,0 \} = \frac{6}{8} E\{1,1 \} \) (Table 1). So it is impossible to find a conical combination of \( \min(|A \cap B|, i) \) that equals \( f_5 \).