Submodularity
In Machine Learning and Artificial Intelligence

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Abstract

In this manuscript, we offer a gentle review of submodularity and supermodularity and their properties. We offer a plethora of submodular definitions; a full description of a number of example submodular functions and their generalizations; example discrete constraints; a discussion of basic algorithms for maximization, minimization, and other operations; a brief overview of continuous submodular extensions; and some historical applications. We then turn to how submodularity is useful in machine learning and artificial intelligence. This includes summarization, and we offer a complete account of the differences between and commonalities amongst sketching, coresets, extractive and abstractive summarization in NLP, data distillation and condensation, and data subset selection and feature selection. We discuss a variety of ways to produce a submodular function useful for machine learning, including heuristic hand-crafting, learning or approximately learning a submodular function or aspects thereof, and some advantages of the use of a submodular function as a coreset producer. We discuss submodular combinatorial information functions, and how submodularity is useful for clustering, data partitioning, parallel machine learning, active and semi-supervised learning, probabilistic modeling, and structured norms and loss functions.¹

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Many, if not most, problems in machine learning involve some form of optimization. The problem of "learning" itself can be seen simply as a problem of optimizing a specified objective over a set of parameters where the objective is also parameterized by data. The typical example is \( \min_\theta J_\theta(D) \) where \( \theta \) is a vector of continuous valued parameters and \( D \) is a sampled (training) dataset. As is widely known, convex optimization is an important mathematical strategy used in machine learning theory and by many machine learning applications. Many seemingly disparate optimization problems such as nonlinear classification [SS02], clustering [LG07], and dimensionality reduction [WPS05] can be cast as convex programs. When minimizing a convex loss function, we can be assured that efficiently finding an optimal solution, even for large problems, is feasible. Convex optimization is a structural property of the objective in the space of inherently continuous optimization problems.

There are many problems in machine learning, however, that are inherently discrete, where optimization must occur not over a continuous but rather a discrete parameter space. In this case, the objective provides a value over a countable or finite (although often exponentially large) number of possibilities. For example, given a set of features that potentially could be used as the input to a classifier, how should one choose a useful subset? If there are \( m \) features, there are \( 2^m \) possible subsets, far too many to consider them all in an exhaustive search. This is the standard feature selection problem in machine learning for which there are many possible solutions. Rather than select features, we might wish to select a subset of the training data. The reasons for doing so abound: the training data might be too large, or it might be redundant, and hence it will be unnecessarily costly to use all of it. One option is to select a random subset, but this can miss corner cases. Perhaps there is a better way to select a subset that is good in some way, i.e., that is guaranteed to faithfully represent all of the data. Another example is human labeling and annotating a training dataset, a process that is often a costly, time-consuming, tedious, and error-prone endeavor. Rather than labeling all of the data, one can perhaps choose a good subset on which having the labels would be just as good as having the labels on the whole. Batch active learning is an example of this.

As yet another example: how should one choose the structure, e.g., the width and depth, of a deep neural network? Again, this is an important problem and can be seen as a generalization of feature selection since we are considering not only all possible subsets of the input feature set, but all sets of possible hidden units in each layer of a DNN, and all possible number of layers, a countably infinite space to consider, in theory. Despite the difficulty presented by the combinatorial exposition of possibilities, researchers have endeavored to provide useful solutions, examples being all of the work on recent AutoML and NAS methods. The lottery ticket hypothesis, stating that any neural network can be approximated sufficiently well by selecting the right subnetwork (i.e., a subset of hidden units and weights) out of a much larger random network, is enticing, but how could one master the finite but still combinatorial explosion of possible subnetworks?
To offer still another example of discrete optimization in ML, consider the case when one wishes to compute MAP inference in a probabilistic model: \( \arg\max_y p(y|x) \) where \( y \) is a multivariate integer-valued variable. Performing such inference naively is clearly, in the size of \( y \), an exponential cost prospect. How can one do this efficiently? This problem is essentially the same as the semantic image segmentation problem described in other chapters of the book, where \( x \) is a set of pixels and \( y \) is a set of integer labels one for each pixel. One way to tame the complexity of this problem is to assume that certain factorization properties are true of \( p(y|x) \) which allows the use of the distributed law, and this is one of the purposes of graphical models (i.e., to describe what factorization properties are active). This allows exact or (more often) approximate solutions to be feasibly and practically computed. However, what if the factorization properties assumed of \( p(y|x) \) that enable tractable exact or approximate computation are inaccurate or undesirable? Does this leave us with no recourse to proceed?

Lastly, while it is known that continuous representations of discrete phenomena (such as words, sentences, or even knowledge representation and logic clauses in the domain of NLP) are useful and there has been much recent research on this topic, at some point we must eventually make a final crisp decision. For example, in a speech recognition system, we need a final single word string hypothesis corresponding to what was spoken. In an autonomous vehicle, we need at some point to decide whether to stop, go, turn left, right, or to continue forward. In financial investing, we need to decide to buy, sell, or do nothing. These are all discrete decisions that any machine learning system must eventually deal with.

Regardless of the approach taken to solve these problems, we see how they all require a form of discrete optimization for their solution. Many other machine learning problems are also inherently and fundamentally discrete. It is thus useful to study machine learning structures that themselves are inherently discrete. It is also important for these structures to be easily applicable to many different problems, and also that are amenable to efficient combinatorial optimization strategies, even when the solution space may be exponential in the problem size. Submodular functions fit this bill well.

Submodularity has an extremely simple definition. However, the “simplest things are often the most complicated to understand fully” [Sam74], and while submodularity has been studied extensively over the years, it continues to yield new and surprising insights and properties, some of which are extremely relevant to data science, machine learning, and artificial intelligence. A submodular function operates on subsets of some finite ground set, \( V \). Finding a guaranteed good subset of \( V \) would ordinarily require an amount of computation exponential in the size of \( V \). Submodular functions, however, have certain properties that make optimization either tractable or approximable where otherwise neither would be possible. The properties are quite natural, however, so submodular functions are both flexible and widely applicable to real problems. Submodularity involves an intuitive and natural diminishing returns property, stating that adding an element to a smaller set helps more than adding it to a larger set. Like convexity, submodularity allows one to efficiently find provably optimal or near-optimal solutions. In contrast to convexity, however, where little regarding maximization is guaranteed, submodular functions can be both minimized and (approximately) maximized. Submodular maximization and minimization, however, require very different algorithmic solutions and have quite different applications. It is sometimes said that submodular functions are a discrete form of convexity. This is not quite true, as submodular functions are like both convex and concave functions, but also have properties that are similar simultaneously to both convex and concave functions at the same time, but then some properties of submodularity are neither like convexity nor like concavity. Convexity and concavity, for example, can be conveyed even as univariate functions. This is impossible for submodularity, as submodular functions are defined based only on the response of the function to changes amongst different variables in a multidimensional discrete space (this is discussed a bit more in the context of DR-submodularity below).

There is a growing interest in submodularity in machine learning, as witnessed by the increasing number of such articles seen in recent years at machine learning conferences, and some of these will be surveyed in Section 3. Before we do, we start the next section by describing submodularity in as simple a way as possible.
2 Intuition, Examples, and Background

Let us define a set function \( f : 2^V \rightarrow \mathbb{R} \) as one that assigns a value to every subset of \( V \). The notation \( 2^V \) is the power set of \( V \), and has size \( 2^{|V|} \), which means that \( f \) lives in space \( \mathbb{R}^{2^{|V|}} \) -- i.e., since there are \( 2^n \) possible subsets of \( V \), \( f \) can return \( 2^n \) distinct values. We use the notation \( X \cup v \) as shorthand for \( X \cup \{v\} \). Also, the value of an element in a given context is so widely used a concept, we have a special notation for it --- the incremental value.\footnote{The notation \( f(v|X) \) is the value of element \( v \) if you already have \( X \). We also define the gain of set \( X \) in the context of \( Y \) as \( f(X|Y) = f(X \cup Y) - f(Y) \).}

\[
\text{f(v|X) = f(X + v) - f(X) is the incremental value of gaining friend v if you already have the set of friends X. Submodularity says that the incremental value of any friend v decreases the more friends you acquire. So if you increase your friend set from X to Y \( \subseteq X \), then the incremental value of friend v cannot increase. If you have a friend Taylor, then Taylor would be much more valuable to you as your first friend than they would be if you already had Emerson, Tatum, Bellamy, Leon, and Tatum as friends. In general, submodular functions are those that satisfy the property of diminishing returns. This means that the incremental “value” or “gain” of \( v \) decreases as the context in which \( v \) is considered grows from \( X \) to \( Y \).}
\]

2.0.1 The Value of Friendship

To introduce submodularity, we begin with the value of friendship. Let’s say that \( f(X) \) measures the value of a set \( X \) of friends and \( v \) is a friend that you do not yet have. Then \( f(X + v) \) is the value once you have gained friend \( v \) and \( f(v|X) = f(X + v) - f(X) \) is the incremental value of gaining friend \( v \) if you already have the set of friends \( X \). Submodularity says that the incremental value of any friend \( v \) decreases the more friends you acquire. So if you increase your friend set from \( X \) to \( Y \subset X \), then the incremental value of friend \( v \) cannot increase. If you have a friend Taylor, then Taylor would be much more valuable to you as your first friend than they would be if you already had Emerson, Tatum, Bellamy, Leon, and Tatum as friends. In general, submodular functions are those that satisfy the property of diminishing returns. This means that the incremental “value” or “gain” of \( v \) decreases as the context in which \( v \) is considered grows from \( X \) to \( Y \).

2.0.2 Coffee, Lemon, Milk, Tea

As our next example, we will explore the manner in which the value of everyday items may interact and combine, namely coffee, lemon, milk, and tea. Consider the value relationships amongst the four items coffee (c), lemon (l), milk (m), and tea (t) as shown in Figure 1. Suppose you just woke up, and there is a function \( f : 2^V \rightarrow \mathbb{R} \) that provides the average valuation for any subset of the items in V where \( V = \{c, l, m, t\} \). You can think of this function as giving the average price a typical person would be willing to pay for any subset of items. Since nothing should cost nothing, we would expect that \( f(\emptyset) = 0 \). Clearly, one needs either coffee or tea in the morning, so \( f(c) > 0 \) and \( f(t) > 0 \), and coffee is usually more expensive than tea, so that \( f(c) > f(t) \) pound for pound. Also more items cost more, so that, for example, \( 0 < f(c) < f(c, m) < f(c, m, t) < f(c, l, m, t) \). Thus, the function \( f \) is strictly monotone, or \( f(X) < f(Y) \) whenever \( X \subseteq Y \).

The next thing we note is that coffee and tea may substitute for each other -- they both have the same effect, waking you up. Once you have tea you do not need as much coffee, and vice versa. They are mutually redundant, and they decrease each other’s value since once you have had a cup of coffee, a cup of tea is less necessary and less desirable. Thus, \( f(c, t) < f(c) + f(t) \), which is known as a subadditive relationship, the whole is less than the sum of the parts. On the other hand, some items complement each other. For example, milk and coffee are better combined together than when both are considered in isolation, or \( f(m, c) > f(m) + f(c) \), a superadditive relationship, the whole is more than the sum of the parts. A similar superadditive relationship exists between milk and tea \( f(m, t) > f(m) + f(t) \) as well as lemon and tea \( f(l, t) > f(l) + f(t) \). A few of the items do not affect each other’s price. For example, lemon and milk cost the same together as apart, so \( f(l, m) = f(l) + f(m) \), an additive or modular relationship --- such a relationship is perhaps midway between a subadditive and a superadditive relationship and can be seen as a form of independence. A similar thing is true for lemon and coffee \( f(l, c) = f(l) + f(c) \).

Things become more interesting when we consider three or more items together. For example, once you have tea, lemon becomes less valuable when you acquire milk since there might be those that prefer milk to lemon in their tea. Similarly, milk becomes less valuable once you have acquired lemon since there are those who prefer lemon in their tea to milk. So, once you have tea, lemon and milk are substitutive, you would never use both as the lemon would only curdle the milk. These are submodular relationships, \( f(l|m, t) < f(l|t) \) and \( f(m|l, t) < f(m|l) \) each of which implies that \( f(l, t) + f(m, t) > f(l, m, t) + f(t) \). The value of lemon (respectively milk) with tea decreases in the larger context of having milk (respectively lemon) with tea, typical of submodular relationships.
with both milk and coffee, since lemon is of no more use with coffee and milk as it is with just milk. This presence of tea again reduces the value of coffee. Lemon alone does not affect the price of coffee, but tea and lemon are additive (modular, or independent). We next see a four-dimensional hypercube (tesseract) showing all of the value relationships described in the text. The four-dimensional hypercube is also shown as a lattice (on the right) showing the same relationships as well as two (red and green, also shown in the tesseract) of the eight three-dimensional cubes contained within.

A submodular relationship also exists over coffee, milk, and tea. Once we have milk, then the presence of tea decreases the value of coffee again since coffee and tea are substitutes perhaps even more so with milk. This means that \( f(c|m, t) < f(c|m) \) and \( f(t|c, m) < f(t|m) \), implying \( f(m, t) + f(m, c) > f(m, c, t) + f(m) \).

Another submodular relationship exists over coffee, lemon, and tea. Once you have lemon, then the presence of tea again reduces the value of coffee. Lemon alone does not affect the price of coffee, but tea and lemon perhaps renders coffee undesirable. The relationships are \( f(c|t, l) < f(c|l) \) and \( f(t|c, l) < f(t|l) \), implying \( f(l, t) + f(c, l) > f(c, l, t) + f(l) \).

Not all of the items are in a submodular relationship, as sometimes the presence of an item can increase the value of another item. For example, once you have milk, then tea becomes still more valuable when you also acquire lemon, since tea with the choice of either lemon or milk is more valuable than tea with the option only of milk. Similarly, once you have milk, lemon becomes more valuable when you acquire tea, since lemon with milk alone is not nearly as valuable as lemon with tea, even if milk is at hand. This means that \( f(t|m, l) > f(t|m) \) and \( f(l|t, m) > f(l|m) \) implying \( f(l, m) + f(m, l) > f(l, m, t) + f(l) \).

Another supermodular relationship exists over lemon, milk, and tea. The value of milk increases if you have both tea and lemon compared to if you have only lemon, and the value of tea increases if you have both milk and lemon over if you just have lemon, or \( f(m|l, t) > f(m|l) \) and \( f(l|m, t) > f(l|m) \). Other supermodular relationships exist over lemon, milk, and coffee \( f(c, l) + f(l, m) < f(c, l, m) + f(l) \), over coffee, milk, and tea \( f(c, t) + f(c, m) < f(c, m, t) + f(c) \) and \( f(c, t) + f(m, t) < f(c, m, t) + f(c) \), and also over coffee, lemon, and tea \( f(c, t) + f(c, l) < f(c, l, t) + f(c) \).

Some of the triples have a relationship that lies in between submodularity and supermodularity. For example, if you start with milk, then the value of lemon should be no different than if you had started with both milk and coffee, since lemon is of no more use with coffee and milk as it is with just milk. This means that \( f(l|c, m) = f(l|m) \). Similarity, lemon does not improve coffee’s value over having just milk, or \( f(c|l, m) = f(c|m) \). These both imply \( f(c, m) + f(l, m) = f(c, l, m) + f(m) \) which is known as a modular (or additive) relationship. These are actually conditionally modular relationships since we are measuring the value relationships between lemon and coffee in the presence of milk.

In the current case, as mentioned above, lemon and coffee are already additive when considered alone. In other cases, items that are additive alone, e.g., milk and lemon, might have interactive values in a context, e.g., milk and lemon when considered in the context of tea where the relationship becomes substitutive or submodular. This is a particular type of v-structure that is representable with Bayesian

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**Figure 1:** The value relationships between coffee \( (c) \), lemon \( (l) \), milk \( (m) \), and tea \( (t) \). On the left, we first see a simple square showing the relationships between coffee and tea and see that they are substitutive (or submodular). In this, and all of the shapes, the vertex label set is indicated in curly braces and the value at that vertex is a blue integer in a box. We next see a three-dimensional cube that adds lemon to the coffee and tea set. We see that tea and lemon are complementary (supermodular), but coffee and lemon are additive (modular, or independent). We next see a four-dimensional hypercube (tesseract) showing all of the value relationships described in the text. The four-dimensional hypercube is also shown as a lattice (on the right) showing the same relationships as well as two (red and green, also shown in the tesseract) of the eight three-dimensional cubes contained within.
networks, depicted as $m \rightarrow t \leftarrow l$, where $m$ and $l$ are unconditionally independent but conditionally dependent. Here, however, the dependence need not be statistical and instead can be combinatorial. Another conditionally modular relationship is coffee and lemon in the context of tea, where we would expect that $f(c, t) + f(l, t) = f(c, l, t) + f(t)$.

We have asked for a set of relationships amongst various subsets of the four items $V = \{c, l, m, t\}$, Is there a function that offers a value to each $X \subseteq V$ that satisfies all of the above relationships? Figure 1 in fact shows such a function. On the left, we see a two-dimensional square whose vertices indicate the values over subsets of $\{c, l\}$ and we can quickly verify that the sum of the blue boxes on north-west (corresponding to $f(\{c\})$) and south-east corners (corresponding to $f(\{l\})$) is greater than the sum of the north-east and south-west corners, expressing the required submodular relationship. Next on the right is a three-dimensional cube that adds the relationship with lemon. Now we have six squares, and we see that the values at each of the vertices all satisfy the above requirements --- we verify this by considering the valuations at the four corners of every one of the six faces of the cube. Since $|V| = 4$, we need a four-dimensional hypercube to show all values, and this may be shown in two ways. It is first shown as a tesseract, a well-known three-dimensional projection of a four-dimensional hypercube. In the figure, all vertices are labeled both with subsets of $V$ as well as the function value $f(X)$ as the blue number in a box. The inner three-dimensional cube in the tesseract is the same as the cube second from left, and the outer three-dimensional cube in the tesseract includes the interactions with milk. Overall, there are eight three-dimensional cubes within the tesseract, each with six faces. The figure on the right shows a lattice version of the four-dimensional hypercube, where corresponding three-dimensional cubes are shown in green and red. It can be verified that the values at the vertices, even though they consist only of integers from 0 through 9, satisfy all of the aforementioned subadditive, superadditive, submodular, supermodular, and modular relationships amongst subsets of items.

We thus see that a set function is defined for all subsets of a ground set, and that they correspond to valuations at all vertices of the hypercube. For the particular function over valuations of subsets of coffee, lemon, milk, and tea, we have seen submodular, supermodular, and modular relationships all in one function. Therefore, the overall function $f$ defined in Figure 1 is neither submodular, supermodular, nor modular. For combinatorial auctions, there is often a desire to have a diversity of such manners of relationships [LLN06] --- representation of these relationships can be handled by a difference of submodular functions [NB05; IB12] or a sum of a submodular and supermodular function [BB18] (further described below). Nevertheless, it is useful to demonstrate submodular and supermodular relationships amongst particular subsets of everyday items. In machine learning, however, most of the time we are interested in functions that are submodular (or modular, or supermodular) everywhere, over all subsets. The next example will describe a famous example of such a pure submodular function.

### 2.0.3 Entropy

Our next example of submodularity uses a concept that is likely familiar to many machine learning scientists, namely entropy, which measures the uncertainty or the information in a set of random variables. Suppose we are given a set of $n$ discrete random variables $R_1, R_2, \ldots, R_n$. The set $V = \{1, 2, \ldots, n\}$ is an index set, and any subset $A \subseteq V$ of integers can be used to index a subset of random variables. Thus, if $A = \{i_1, i_2, \ldots, i_k\} \subseteq V$, then $R_A = \{R_{i_1}, R_{i_2}, \ldots, R_{i_k}\}$. Given a probability distribution $p$ over $R_V$, the entropy of a set $A$ of random variables is defined as $H(R_A) = -\sum_{r_A} p(r_A) \log p(r_A)$. We note that the number of terms in the summation is exponential in the set size $|A|$. There are a number of properties that are known to be true of the entropy function, and they were established by Shannon back in 1948. The first is that the entropy is non-negative, i.e., $H(R_A) \geq 0$ for any $A$. The second is monotonicity, i.e., for sets $A \subseteq B$, we have that $H(R_A) \leq H(R_B)$. This means that more random variables cannot possess less information. The third, and perhaps most important property of entropy is equivalent to submodularity. The conditional mutual information between two sets $A$ and $B$ of random variables given a third set $C$, all three of which are mutually disjoint, is defined as $I(R_A; R_B|R_C) = \sum_{r_A, r_B, r_C} p(r_A, r_B, r_C) \log \frac{p(r_A, r_B, r_C)}{p(r_A, r_B)p(r_C)}$. The conditional mutual information can be expressed in terms of the entropy, $I(R_A; R_B|R_C) = H(R_A, R_C) + H(R_B, R_C) - H(R_A, R_B, R_C) - H(R_C)$. A well-known property is that the conditional mutual information is non-negative, i.e., $I(R_A; R_B|R_C) \geq 0$.

We can view this inequality in a slightly different way. First, for any set $X \subseteq V$, we define entropy as a set function $f(X) = H(R_X)$, which gives the entropy of the set of random variables indexed by $X$. Then if
we set \( X = A \cup C, Y = B \cup C \), then the above inequality about the non-negativity of mutual information becomes \( f(X) + f(Y) - f(X \cup Y) = f(X \cap Y) \geq 0 \), which is exactly the condition for the submodularity of the set function (see below). Thus, the Shannon entropy function is submodular when seen as a function of subsets of random variables. Statement equivalent to the submodularity of the Shannon entropy function was implied back in Shannon’s paper [Sha48] and made explicit in [McG54]. These inequalities therefore became known, in the information theory community, as the Shannon inequalities [Yeu91; ZY97; ZY98].

### 2.1 Submodular Basic Definitions

For a function to be submodular, it must satisfy the submodular relationship for all subsets. We arrive at the following definition.

**Definition 2.1 (Submodular Function).** A given set function \( f : 2^V \rightarrow \mathbb{R} \) is submodular if for all \( X, Y \subseteq V \), we have the following inequality:

\[
f(X) + f(Y) \geq f(X \cup Y) + f(X \cap Y)
\]

There are also many other equivalent definitions of submodularity some of which are more intuitive and easier to understand. For example, submodular functions are those set functions that satisfy the property of diminishing returns. If we think of a function \( f(X) \) as measuring the value of a set \( X \) that is a subset of a larger set of data items \( X \subseteq V \), then the submodular property means that the incremental “value” of adding a data item \( v \) to set \( X \) decreases as the size of \( X \) grows. This gives us a second classic definition of submodularity.

**Definition 2.2 (Submodular Function via Diminishing Returns).** A given set function \( f : 2^V \rightarrow \mathbb{R} \) is submodular if for all \( X, Y \subseteq V \), where \( X \subseteq Y \) and for all \( v \not\in Y \), we have the following inequality:

\[
f(X) + f(v) - f(X) \geq f(Y) + f(v) - f(Y) \tag{2}
\]

The property that the incremental value of lemon with tea is less than the incremental value of lemon once milk is already in the tea is equivalent to Equation (1) if we set \( X = \{m, t\} \) and \( Y = \{l, t\} \) (i.e. \( f(m, t) + f(l, t) > f(l, m, t) + f(t) \)). It is naturally also equivalent to Equation (2) if we set \( X = \{t\}, Y = \{m, t\} \), and with \( v = l \) (i.e., \( f(l|m, t) < f(l|t) \)). The function listed in Figure 1 is not submodular for all subsets as mentioned above. The entropy function, however, seen as a function of a set of random variables, is submodular over all subsets, and this is widely known as the “further conditioning reduces entropy” property of the entropy function.

It is not hard to see how Equation (2.1) and Equation (2.2) are mathematically identical, as is done in the following:

**Theorem 2.1.** Given function \( f : 2^V \rightarrow \mathbb{R} \), then

\[
f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \text{ for all } A, B \subseteq V \tag{Eq. (2.1)}
\]

if and only if

\[
f(v|X) \geq f(v|Y) \text{ for all } X \subseteq Y \subseteq V \text{ and } v \not\in Y \tag{Eq. (2.2)}
\]

**Proof.** Eq. (2.1)⇒Eq. (2.2): Set \( A \leftarrow X \cup \{v\}, B \leftarrow Y \). Then \( A \cup B = Y \cup \{v\} \) and \( A \cap B = X \) and \( f(A) - f(A \cap B) \geq f(A \cup B) - f(B) \) implies Eq. (2.2).

Eq. (2.2)⇒Eq. (2.1): Order \( A \setminus B = \{v_1, v_2, \ldots, v_r\} \) arbitrarily. For \( i \in [r] \),

\[
f(v_i|A \cap B \cup \{v_1, v_2, \ldots, v_{i-1}\}) \geq f(v_i|B \cup \{v_1, v_2, \ldots, v_{i-1}\}).
\]

Applying telescoping summation to both sides, we get:

\[
\sum_{i=1}^{r} f(v_i|A \cap B \cup \{v_1, v_2, \ldots, v_{i-1}\}) \geq \sum_{i=1}^{r} f(v_i|B \cup \{v_1, v_2, \ldots, v_{i-1}\})
\]

\[
\Rightarrow f(A) - f(A \cap B) \geq f(A \cup B) - f(B)
\]

\qed
There are many different ways to define submodularity. Theorem 2.2 gives a list of equivalencies --- if any one of the equations are true as stated, then the function is submodular.

**Theorem 2.2 (The Many Definitions of Submodularity).** Given a function \( f : 2^V \rightarrow \mathbb{R} \), and the gain function defined as \( f(R|S) = f(R \cup S) - f(S) \), for any sets \( S, R \subseteq V \), the following equations are equivalent. In other words, any one of them can be used as the definition of a submodular function.

\[
\begin{align*}
    f(A) + f(B) &\geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V & (\text{Classic}) \quad (1) \\
    f(v|S) &\geq f(v|T), \quad \forall S \subseteq T \subseteq V, \quad \forall v \in V \setminus T & (\text{Dim. Returns}) \quad (2) \\
    f(v|S) &\geq f(x|S \cup \{y\}), \quad \forall S \subseteq V, \quad \forall x \in V \setminus (S \cup \{y\}) & (\text{Four Points}) \quad (3) \\
    f(C|S) &\geq f(C|T), \quad \forall S \subseteq T \subseteq V, \quad \forall C \subseteq V \setminus T & (\text{Group Dim. Returns}) \quad (4) \\
    f(A \cup B|A \cap B) &\leq f(A|A \cap B) + f(B|A \cap B), \quad \forall A, B \subseteq V & (\text{Conditional Subadditivity}) \quad (5) \\
    f(T) &\leq f(S) + \sum_{v \in T \setminus S} f(v|S) \quad \forall S \subseteq V \setminus T & (\text{Union ULB}) \quad (6) \\
    f(T) &\leq f(S) + \sum_{v \in T \setminus S} f(v|S), \quad \forall S \subseteq T \subseteq V & (\text{Union UB}) \quad (7) \\
    f(T) &\leq f(S) + \sum_{v \in T \setminus S} f(v|S \cap T) \quad \forall S \subseteq T \subseteq V & (\text{Intersection ULB}) \quad (8) \\
    f(T) &\geq f(S) - \sum_{v \in S \setminus T} f(v|S \setminus \{v\}), \quad \forall T \subseteq S \subseteq V & (\text{Intersection UB}) \quad (9) \\
    f(T) &\leq f(S) + \sum_{v \in T \setminus S} f(v|S \cap T) \quad \forall T \subseteq S \subseteq V & (\text{Union/Intersection}) \quad (10)
\end{align*}
\]

While entropy as seen above is submodular, there are many other functions as well, some of which we examine below. We first point out that there are non-negative (i.e., \( f(A) \geq 0, \forall A \)), monotone non-decreasing (i.e., \( f(A) \leq f(B) \) whenever \( A \subseteq B \)) submodular functions that are not entropic [Yeu91; ZY97; ZY98], so submodularity is not just a trivial restatement of the class of entropy functions. When a function is monotone non-decreasing, submodular, and normalized so that \( f(\emptyset) = 0 \), it is often referred to as a polymatroid function. Thus, while the entropy function is a polymatroid function, it does not encompass all polymatroid functions even though all polymatroid functions satisfy the properties Claude Shannon mentioned as being natural for an “information” function (see Section 3.2). Most polymatroid functions can be seen as a form of dispersion, diversity, or information function, in that they tend to give high valuation to sets \( A \), of a given size, that have a lot of diversity (a high amount of information about \( V \)), and tend to give low value to sets, of the same size, that are more homogeneous (a low amount of information about \( V \)). The entropy function is a good example of this, where diversity over a set of random variables is determined by the degree to which the set of random variables are statistically independent and the degree to which they have high marginal entropy.

A supermodular function has the following (reversed inequality relative to submodularity) definition:

**Definition 2.3 (Increasing Returns).** A given set function \( f : 2^V \rightarrow \mathbb{R} \) is supermodular if for all \( X, Y \subseteq V \), where \( X \subseteq Y \) and for all \( v \notin Y \), we have the following inequality:

\[
f(X + v) - f(X) \leq f(Y + v) - f(Y) \quad (11)
\]

We can alternatively define supermodularity analogous to Definition 2.1, where we say the function \( f \) is supermodular if \( f(X) + f(Y) \leq f(X \cup Y) + f(X \cap Y) \) for all arguments.
Alternatively, a function $f$ is supermodular if and only if $-f$ is submodular. If a function is both submodular and supermodular, it is known as a modular function. It is always the case that modular functions may take the form of a vector-scalar pair $(m, c)$ where $m : 2^V \to \mathbb{R}$ and where $c \in \mathbb{R}$ is a constant, and where for any $A \subseteq V$, we have that $m(A) = c + \sum_{v \in A} m_v$. If the modular function is normalized, so that $m(\emptyset) = 0$, then $c = 0$ and the modular function can be seen simply as a vector $m \in \mathbb{R}^V$. Hence, we sometimes say that the modular function $x \in \mathbb{R}^V$ offers a value for set $A$ as the partial sum $x(A) = \sum_{v \in A} x(v)$. Many combinatorial problems use modular functions as objectives. For example, the graph cut problem uses a modular function defined over the edges, judges a cut in a graph as the modular function applied to the edges that comprise the cut.

As can be seen from the above, and by considering Figure 1, a submodular function, and in fact any set function, $f : 2^V \to \mathbb{R}$ can be seen as a function defined only on the vertices of the $n$-dimensional unit hypercube $[0,1]^n$. Given any set $X \subseteq V$, we define $1_X \in \{0,1\}^V$ to be the characteristic vector of set $X$ defined as $1_X(v) = 1$ if $v \in X$ and $1_X(v) = 0$ otherwise. This gives us a way to map from any set $X \subseteq V$ to a binary vector $1_X$. We also see that $1_X$ is itself a modular function since $1_X \in \{0,1\}^V \subset \mathbb{R}^V$.

A submodular function is not defined using relationships only between pairs of objects like in a typical weighted graph where every edge connects two vertices. Rather, a submodular function provides a distinct value for every unique subset $X \subseteq V$, and the value $f(X)$ need not be a function of the values of pairs of elements $f(i,j)$ for $i,j \in X$. Most generally, a submodular function requires the specification of $2^n$ distinct parameters. To compare a submodular function with a graphical model, for example, a submodular function (most generally) corresponds to a single clique over a set of $n$ variables. Such a graphical model, which normally encodes factorization properties via graph separation properties, would have no factorization properties since nothing is separated in a clique. It is for this reason that submodular functions can be seen to be a form of “anti-graphical” model. In other words, submodular/supermodular functions and graphical models describe distinct properties --- a graphical model depicts who directly interacts with whom while submodular (or supermodular) function states the manner that a group of items may interact amongst themselves. Both graphical models and submodular functions are useful, and they are in fact complementary, since we can use a graphical model to decompose how a submodular function is formed. As a simple example, suppose $V = \{v,w,u,x\}$ and we form the function $f(X) = \sqrt{|X \cap \{v,w\}|} + \sqrt{|X \cap \{w,u\}|} + \sqrt{|X \cap \{u,x\}|}$. Then, not only is function submodular (see below for why), it abides by the rules of a chain graphical model $v - w - u - x$. That is, a graphical model describes which variables may or may not directly interact with each other depending on the presence or absence of edges in a graph, a submodular (or supermodular) function specifies how variables interact.

Submodular functions share a number of properties in common with both convex and concave functions [Lov83], including wide applicability, generality, multiple representations, and closure under a number of common operators (including mixtures, truncation, complementation, and certain convolutions). There is one important submodular closure property that we state here --- that is that if we take non-negative weighted (or conical) combinations of submodular functions, we preserve submodularity. In other words, if we have a set of $k$ submodular functions, $f_i : 2^V \to \mathbb{R}$, $i \in [k]$, and we form $f(X) = \sum_{i=1}^k \omega_i f_i(X)$ where $\omega_i \geq 0$ for all $i$, then Definition 2.1 immediately implies that $f$ is also submodular. When we consider Definition 2.1, we see that submodular functions live in a cone in $2^n$-dimensional space defined by the intersection of an exponential number of half-spaces each one of which is defined by one of the inequalities of the form $f(X) + f(Y) \geq f(X \cup Y) + f(X \cap Y)$. Each submodular function is therefore a point in that cone. It is therefore not surprising that taking conical combinations of such points stays within this cone.

### 2.2 Example Submodular Functions

As mentioned above, there are many functions that are submodular besides entropy. Perhaps the simplest such function is $f(A) = \sqrt{|A|}$ which is the composition of the square-root function (which is concave) with the cardinality $|A|$ of the set $A$. The gain function is $f(A + v) - f(A) = \sqrt{k+1} - \sqrt{k}$ if $|A| = k$, which we know to be a decreasing in $k$, thus establishing the submodularity of $f$. In fact, if $\phi : \mathbb{R} \to \mathbb{R}$ is any concave function, then $f(A) = \phi(|A|)$ will be submodular for the same reason. Generalizing this

---

2While we will not be extensively discussing supermodular functions in this section, $f(A) = \phi(|A|)$ is supermodular for any convex function $\phi$. 

9
slightly further, a function defined as \(f(A) = \phi(\sum_{a \in A} m(a))\) is also submodular, whenever \(m(a) \geq 0\) for all \(a \in V\). This yields a composition of a concave function with a modular function \(f(A) = \phi(m(A))\) since \(\sum_{a \in A} m(a) = m(A)\). We may take sums of such functions as well as add a final modular function without losing submodularity, leading to \(f(A) = \sum_{u \in U} \phi_u(\sum_{a \in A} m_u(a)) + \sum_{a \in A} m_a(a)\) where \(\phi_u\) can be a distinct concave function for each \(u\), \(m_u(a)\) is a non-negative real value for all \(u\) and \(a\), and \(m_a(a)\) is an arbitrary real number. Therefore, \(f(A) = \sum_{u \in U} \phi_u(m_u(A)) + m_a(A)\) where \(m_u\) is a \(u\)-specific non-negative modular function and \(m_a\) is an arbitrary modular function. Such functions are sometimes known as feature-based submodular functions [BB17] because \(U\) can be a set of non-negative features (in the machine-learning “bag-of-words” sense) and this function measures a form of dispersion over \(A\) as determined by the set of features \(U\).

A function such as \(f(A) = \sum_{u \in U} \phi_u(m_u(A))\) tends to award high diversity to a set \(A\) that has a high valuation by a distinct set of the features \(U\). The reason is that, due to the concave nature of \(\phi_u\), any addition to the argument \(m_u(A)\) by adding, say, \(v\) to \(A\) would diminish as \(A\) gets larger. In order to produce a set larger than \(A\) that has a much larger valuation, one must use a feature \(u' \neq u\) that has not yet diminished as much.

Facility location is another well-known submodular function --- perhaps an appropriate nickname would be the “\(k\)-means of submodular functions,” due to its applicability, utility, ease-of-use (it needs only an affinity matrix), and similarity to \(k\)-medoids problems. The facility location function is defined using an affinity matrix as follows: \(f(A) = \sum_{v \in V} \max_{a \in A} \text{sim}(a,v)\) where \(\text{sim}(a,v)\) is a non-negative measure of the affinity (or similarity) between element \(a\) and \(v\). Here, every element \(v \in V\) must have a representative within the set \(A\) and the representative for each \(v \in V\) is chosen to be the element \(a \in A\) most similar to \(v\). This function is also a form of dispersion or diversity function because, in order to maximize it, every element \(v \in V\) must have some element similar to it in \(A\). The overall score is then the sum of the similarity between each element \(v \in V\) and \(v\)’s representative. This function is monotone (since as \(A\) includes more elements to become \(B \supseteq A\), it is possible only to find an element in \(B\) more similar to a given \(v\) than an element in \(A\)).

While the facility location looks quite different from a feature-based function, it is possible to precisely represent any facility location function with a feature-based function. One way to see this is to consider \(\max_{a \in A} x_a = \lim_{y \to 0} \frac{1}{y} \log(\sum_{a \in A} \exp(y x_a))\), for non-negative values \(x_a\). Thus, the \(\max\) function acts as a kind of sharp concave function. Alternatively, we can capture the facility location directly by a feature-based function, term by term, by sorting the individual modular functions. Consider just \(\max_{a \in A} x_a\) and, without loss of generality, assume that \(0 \leq x_1 \leq x_2 \leq \cdots \leq x_n\). Then \(\max_{a \in A} x_a = \sum_{i=1}^{n} y_i \min(|A \cap \{i, i+1, \ldots, n\}|, 1)\) where \(y_i = x_i - x_{i-1}\) and we set \(x_0 = 0\). We note that this is a sum of weighted concave composed with modular functions since \(\min(\alpha, 1)\) is concave in \(\alpha\), and \(|A \cap \{i, i+1, \ldots, n\}|\) is a modular function in \(A\). Thus, the facility location function, a sum of these, is merely a feature-based function. In fact, since budgeted additive functions [Dev+13] are the same as truncated modular functions (i.e., those that take the form \(f(X) = \min(\alpha, \sum_{v \in X} m(v))\)), we see that a facility location function can be represented by class of functions smaller than feature-based functions.

Feature-based functions, in fact, are quite expressive, and can be used to represent many different submodular functions including set cover and graph-based functions. For example, we can define a set cover function, given a set of sets \(\{U_v \}_{v \in V}\), via \(f(X) = |\bigcup_{v \in X} U_v|\). If \(f(X) = |U|\) where \(U = \bigcup_{v \in V} U_v\) then \(X\) indexes a set that fully covers \(U\). This can also be represented as \(f(X) = \sum_{u \in U} \min(1, m_u(X))\) where \(m_u(X)\) is a modular function where \(m_u(v) = 1\) if and only if \(u \in U_v\) and otherwise \(m_u(v) = 0\). We see that this is a feature-based submodular function since \(\min(1, x)\) is concave in \(x\), and \(U\) is a set of features.

This construct can be used to produce the vertex cover function if we set \(U = V\) to be the set of vertices in a graph, and set \(m_u(v) = 1\) if and only if vertices \(u\) and \(v\) are adjacent in the graph and otherwise \(m_u(v) = 1\). Similarly, the edge cover function can be expressed by setting \(V\) to be the set of edges in a graph, \(U\) to be the set of vertices in the graph, and \(m_u(v) = 1\) if and only edge \(v\) is incident to vertex \(u\).

A generalization of the set cover function is the probabilistic coverage function. Let \(P[B_{u,v} = 1]\) be the probability of the presence of feature (or concept) \(u\) within element \(v\). Here, we treat \(B_{u,v}\) as a Bernoulli random variable for each element \(v\) and feature \(u\) so that \(P[B_{u,v} = 1] = 1 - P[B_{u,v} = 0]\). Then we can define the probabilistic coverage function as \(f(X) = \sum_{u \in U} f_u(X)\) where, for feature \(u\), we have \(f_u(X) = 1 - \prod_{v \in X} (1 - P[B_{u,v} = 1])\) which indicates the degree to which feature \(u\) is “covered” by \(X\). If we set \(P[B_{u,v} = 1] = 1\) if and only if \(u \in U_v\) and otherwise \(P[B_{u,v} = 1] = 0\), then \(f_u(X) = \min(1, m_u(X))\) and the set cover function can be represented as \(\sum_{u \in U} f_u(X)\). We can generalize this in two ways. First, to make it softer
and more probabilistic we allow $P[B_{u,v} = 1]$ to be any number between zero and one. We also allow each feature to have a non-negative weight. This yields the general form of the probabilistic coverage function, which is defined by taking a weighted combination over all features: $f_u(X) = \sum_{u \in X} \omega_u f_u(X)$ where $\omega_u \geq 0$ is a weight for feature $u$. Observe that $1 - \prod_{u \in X} (1 - P[B_{u,v} = 1]) = 1 - \exp(-m_u(X))$ where $m_u$ is a modular function with evaluation $m_u(X) = \sum_{u \in X} \exp(-m_u(X))$ and for $z \in \mathbb{R}$, $\exp(-z)$ is a concave function. Thus, the probabilistic coverage function (and its set cover specialization) is also a feature-based function. A variant of this function utilizes the probability $P[u|v]$ rather than $P[B_{u,v} = 1]$, and while this form is not able to perfectly represent the set cover function, it is useful for many applications, for example when $P[u|v]$ indicates the probability of topic $u$ being present in document $v$.

Another common submodular function is the graph cut function. Here, we measure the value of a subset of $V$ by the edges that cross between a set of nodes and all but that set of nodes. We are given an undirected non-negative weighted graph $G = (V, E, w)$ where $V$ is the set of nodes, $E \subseteq V \times V$ is the set of edges, and $w \in \mathbb{R}^E$ are non-negative edge weights corresponding to symmetric matrix (so $w_{i,j} = w_{j,i}$). For any $e \in E$, we have $e = \{i, j\}$ for some $i, j \in V$ with $i \neq j$, the graph cut function $f : 2^V \rightarrow \mathbb{R}$ is defined as $f(X) = \sum_{i \in X, j \in X} w_{i,j}$ where $w_{i,j} \geq 0$ is the weight of edge $e = \{i, j\}$ ($w_{i,j} = 0$ if the edge does not exist), and where $\overline{X} = V \setminus X$ is the complement of set $X$. Notice that we can write the graph cut function as follows:

\[
f(X) = \sum_{i \in X, j \in \overline{X}} w_{i,j} = \sum_{i,j \in V} w_{i,j} \mathbf{1}\{i \in X, j \in \overline{X}\}
\]

\[
= \frac{1}{2} \sum_{i,j \in V} w_{i,j} \left[ \mathbf{1}\{i \in X, j \in \overline{X}\} + \mathbf{1}\{j \in X, i \in \overline{X}\} \right]
\]

\[
= \frac{1}{2} \sum_{i,j \in V} w_{i,j} \left[ \min(|X \cap \{i, j\}|, 1) + \min(|(V \setminus X) \cap \{i, j\}|, 1) \right) - 1
\]

\[
= \frac{1}{2} \sum_{i,j \in V} w_{i,j} \min(|X \cap \{i, j\}|, 1) + \frac{1}{2} \sum_{i,j \in V} w_{i,j} \min(|(V \setminus X) \cap \{i, j\}|, 1) - \frac{1}{2} \sum_{i,j \in V} w_{i,j}
\]

\[
= \tilde{f}(X) + \tilde{f}(V \setminus X) - \tilde{f}(V)
\]

where $\tilde{f}(X) = \frac{1}{2} \sum_{i \in V} w_{i,i} \min(|X \cap \{i\}|, 1)$ (which itself is a form of monotone submodular graph function that, for a set of nodes $X$, returns the sum of edge weights for all edges incident to at least one node in $X$) and where Equation (12) follows due to symmetry. Therefore, since $\min(\alpha, 1)$ is concave, and since $m_{i,j}(X) = |X \cap \{i, j\}|$ is modular, $\tilde{f}(X)$ is submodular for all $i, j$. Also, since $\tilde{f}(X)$ is submodular, so is $\tilde{f}(V \setminus X)$ (in $X$). Therefore, the graph cut function can be expressed as a sum of non-normalized feature-based functions. Note that here the second modular function is not normalized and is non-increasing, and also we subtract the constant $\tilde{f}(V)$ to achieve equality.

We can express the graph cut as a pure feature-based function as described above, as well as allow directed graph cuts, as follows. The indicator $\mathbf{1}\{i \in X, j \in \overline{X}\}$ used above is an inherently directed asymmetric quantity whose directness quality vanished due to the symmetry of $w$. Suppose now it is allowed for $w_{i,j} \neq w_{j,i}$ and we interpret $w_{i,j}$ as the weight of a directed edge from node $i$ to node $j$. An undirected edge is still expressible whenever $w_{i,j} = w_{j,i}$. The general graph cut can then be expressed as follows:

\[
f(X) = \sum_{i \in X, j \in \overline{X}} w_{i,j} = \sum_{i,j \in V} w_{i,j} \mathbf{1}\{i \in X, j \in \overline{X}\}
\]

\[
= \sum_{i,j \in V} w_{i,j} \left[ \min(2 \times \mathbf{1}\{i \in X\} + \mathbf{1}\{j \in X\}, 2) - |X \cap \{i, j\}| \right]
\]

\[
= \sum_{i,j \in V} w_{i,j} \min(m_{i,j}(X), 2) - \sum_{i,j \in V} w_{i,j} |X \cap \{i, j\}|
\]

where $m_{i,j}(X) = \min(2 \times \mathbf{1}\{i \in X\} + \mathbf{1}\{j \in X\}, 2)$ is a non-negative monotone non-decreasing modular function for all $i, j$ and the r.h.s. term is negative modular.
We can slightly generalize the graph cut function to a parameterized form in the following. Let $\lambda = 1$ for now. Then the graph cut can be written as:

$$f(X) = \sum_{i\in X} w_{i,j} = \sum_{i\in X} \left[ \sum_{j\in X} (1 - \lambda) w_{i,j} + \sum_{j\in X} w_{i,j} \right]$$

(20)

$$= \sum_{i\in X, j\in V} w_{i,j} - \lambda \sum_{i\in X, j\in X} w_{i,j} = \sum_{i\in X} w_i - \lambda \sum_{j\in X, i\in X} w_{i,j}$$

(21)

where $w_i$ is the weight of node $i$ (the sum of the weight of edges incident to vertex $i$) and we note that $\sum_{i\in X, j\in X} w_{i,j}$ is a classic supermodular function in $X$ (see Section 2.2.1). Since this takes the form of a modular minus a supermodular function, any value $\lambda \geq 0$ will preserve submodularity, so we consider this a form of generalized graph cut. This generalized form holds for both undirected and directed graph cuts. We leave as an exercise the question of if this can be represented as a feature-based function or not.

One way of viewing the above, when wishing to maximize this function, is to consider $w_{i,j}$ as a similarity value between node $i$ and $j$ in a graph. Then $\sum_{i\in X, j\in X} w_{i,j}$ measures overall how similar the set $X$ is to all of the nodes while $\sum_{i\in X, j\in X} w_{i,j}$ can be viewed as a supermodular redundancy penalty, since it is the sum of pairwise similarities between every node in $X$. We wish for sets that are similar to all the nodes but that are not redundant. Using a negative supermodular function as a redundancy penalty is the approach taken in [LB10a]. If there is an item $j \in V$ that is very similar to many other items, meaning $w_{i,j}$ is very large for all $i$, even when all of the elements are quite different from each other (which implies a strong transitivity relationship would not exist in this case), then maximizing $f(X)$ might choose elements for $X$ only because they are similar to this one element $j$ not because they are similar to many other elements (which ideally is what we would want). The supermodular redundancy penalty does not help in this case since the items being mostly dissimilar to each other would still be granted a small penalty. To limit this from happening, we can modify the first term so that it saturates, and produce a further generalized graph cut function of the form:

$$f(X) = \sum_{j\in V} \min(\sum_{i\in X} w_{i,j}, \alpha \sum_{i\in X} w_{i,j}) - \lambda \sum_{i\in X, j\in X} w_{i,j}$$

(22)

$$= \sum_{j\in V} \min(C_j(X), \alpha C_j(V)) - \lambda \sum_{i\in X, j\in X} w_{i,j}$$

(23)

where $C_j(X) = \sum_{i\in X} w_{i,j}$ is a modular function for all $j$ and $0 \leq \alpha \leq 1$. The minimum function limits the influence that node $j$ has on selecting elements for $X$ to no more than an $\alpha$ fraction of the total possible affinity $j$ has with the remaining nodes. Since we’ve turned the modular function into a feature-based function, submodularity is preserved. In fact, it is sometimes useful to use this function even when $\lambda = 0$, but one should be reminded again that this recovers the standard graph cut function when $\lambda = 1$ and $\alpha = 1$.

Another way to view the graph cut function is to consider the non-negative weights as a modular function defined over the edges. That is, we view $w \in \mathbb{R}_+^E$ as a modular function $w : 2^E \to \mathbb{R}_+$ where for every $A \subseteq E$, $w(A) = \sum_{e \in A} w(e)$ is the weight of the edges $A$ where $w(e)$ is the weight of edge $e$. Then the graph cut function becomes $f(X) = w((a,b) \in E : a \in X, b \in X \setminus X})$. We view $\{(a,b) \in E : a \in X, b \in X \setminus X\}$ as a set-to-set mapping function, that maps subsets of nodes to subsets of edges, and the edge weight modular function $w$ measures the weight of the resulting edges. This immediately suggests that other functions can measure the weight of the resulting edges as well, including non-modular functions. One example is to use a polymatroid function itself leading $h(X) = g((a,b) \in E : a \in X, b \in X \setminus X})$ where $g : 2^E \to \mathbb{R}_+$ is a submodular function defined on subsets of edges. The function $h$ is known as the cooperative cut function, and it is neither submodular nor supermodular in general but there are many useful and practical algorithms that can be used to optimize it [JB16] thanks to its internal yet exposed and thus available to exploit submodular structure.

While feature-based functions are flexible and powerful, there is a strictly broader class of submodular functions, unable to be expressed by feature-based functions, that are related to deep neural networks. Here, we create a recursively nested composition of concave functions with sums of compositions of concave functions. An example is $f(A) = \phi(\sum_{u \in U} w_u \phi_u(\sum_{a \in A} m_{a,u}))$, where $\phi$ is an outer concave function composed
with a feature-based function, with \( m_{u,a} \geq 0 \) and \( \omega_u \geq 0 \). This is known as a two-layer deep submodular function (DSF). A three-layer DSF has the form \( f(A) = \psi(\sum_{c \in C} \omega_c \phi_c(\sum_{a \in A} \omega_{u,a} \phi_u(\sum_{a \in A} m_{u,a}))) \). DSFs strictly expand the class of submodular functions beyond feature-based functions, meaning that there are feature-based functions that cannot [BB17] represent deep submodular functions, even simple ones. For example, the function \( f : 2^V \to \mathbb{R} \) where \( V = \{a, b, c, d, e, f\} \) cannot be represented by a feature-based function.

\[
f(A) = \min\left(\min(|A \cap \{a, b, c, d\}|, 3) + \min(|A \cap \{c, d, e, f\}|, 3), 5\right)
\]

(24)

In fact, the space of representable submodular functions strictly grows with each new layer added to a DSF. DSFs are analogous to deep neural networks, but where the weights may never be negative, and the non-linear activation functions are monotone non-decreasing concave functions, for example \( \min(a, 1) \) or \( \sqrt{a} \). A full discussion is given in [BB17].

### 2.2.1 Example Supermodular Functions

There are also a number of simple functions that are supermodular. Firstly, the feature-based functions mentioned above. That is, a composition of a convex function with a modular function \( g(A) = \psi(m(A)) \) since \( \sum_{a \in A} m(a) = m(A) \). We may take sums of such functions as well without losing supermodularity, leading to \( g(A) = \sum_{u \in U} \psi_u(\sum_{a \in A} m_{u,a}(a)) \) where \( \psi_u \) can be a distinct convex function for each \( u \) and \( m_{u,a} \) is a non-negative real value for all \( u \) and \( a \). This is identical to sums of functions each of which is a convex composed with a modular function \( g(A) = \sum_{u \in U} \psi_u(m_u(A)) \) where \( m_u \) is a \( u \)-specific non-negative modular function.

Another classic submodular function has been known as the sum-sum-dispersion function. It is defined on a square matrix with non-negative entries, specifically \( g(A) = \sum_{a,a' \in A} \text{sim}(a, a') \) where \( \text{sim}(a, a') \) is any non-negative value that expresses the relationship between \( a \) and \( a' \). If \( \text{sim}(a, a') \) is an affinity or similarity score, then \( g(A) \) being large indicates the homogeneity of the set \( A \) since everything with \( A \) is mutually pairwise similar.

### 2.3 Submodular Optimization

As mentioned earlier, machine learning involves (often continuous) mathematical optimization. Submodular functions, while discrete, would not be very useful if it was not possible to optimize over them efficiently. There are many natural problems in machine learning that can be cast as submodular optimization and that can be addressed relatively efficiently.

When one wishes to encourage diversity, information, spread, high complexity, independence, coverage, or dispersion, one usually will maximize a submodular function, in the form of \( \max_{A \subseteq C} f(A) \) where \( C \subseteq 2^V \) is a constraint set, a set of subsets we are willing to accept as feasible solutions (more on this below). For example, \( f \) might correspond to the value of a set of sensor locations in an environment, and we wish to find the best set \( X \subseteq V \) of sensors locations given a fixed upper limit on the number of sensors \( k \). Alternatively, if \( V \) is a set of documents, one might wish to choose a subset \( X \subseteq V \) of documents that act as a good representative of a complete set of documents —— this is a document summarization task. As a third example, if \( V \) is a large training dataset over which it is costly to train a deep neural network, one might wish to find a representative subset \( X \) of size \( k \) to train in as surrogate for \( V \), one that works much better than a uniformly-at-random subset of size \( k \). This is a coreset task. Submodularity is a good general model for such problems because submodular functions act as a form of information function (Section 3.2). Maximizing a submodular function subject to a constraint selects a subset that is non-redundant and thus not wasteful. If we can find a small set that retains most or all of the valuation of the whole (which maximization strives to achieve), we have not lost information as measured by the submodular function, and if the subset is small, it becomes an efficient representation of the information contained in the whole.

Why is submodularity, in general, a good model for diversity? Submodular functions are such that once you have some elements, any other elements not in your possession but that are similar to, explained by, or represented by the elements in your possession become less valuable. Thus, in order to maximize the function, one must choose other elements that are dissimilar to, or not well represented by, the ones you
Figure 2: Far Left: cardinality constrained (to ten) submodular maximization of a facility location function over 1000 points in two dimensions. Similarities are based on a Gaussian kernel \( \text{sim}(a, v) = \exp(-d(a, v)) \) where \( d(\cdot, \cdot) \) is a distance. Selected points are green stars, and the greedy order is also shown next to each selected point. Right three plots: different uniformly-at-random subsets of size ten.

already have. That is, the elements similar to the ones you own are diminished in value relative to their original values, while the elements dissimilar to the ones you have do not have diminished value relative to their original values. Thus, maximizing a submodular function successfully involves choosing elements that are jointly dissimilar amongst each other, which is a definition of diversity. Diversity in general is a critically important aspect in machine learning and artificial intelligence. For example, bias in data science and machine learning can often be seen as some lack of diversity somewhere. Submodular functions have the potential to encourage (and even ensure) diversity, enhance balance, and reduce bias in artificial intelligence.

Note that in order for a submodular function to appropriately model diversity, it is important for it to be instantiated appropriately. Figure 2 shows an example in two dimensions. The plot compares the ten points chosen according to a facility location instantiated with a Gaussian kernel, along with the random samples of size ten. We see that the facility location selected points are more diverse and tend to cover the space much better than any of the randomly selected points, each of which miss large regions of the space and/or show cases where points near each other are jointly selected.

When one wishes for homogeneity, conformity, low complexity, coherence, or cooperation, one will usually minimize a submodular function, in the form of \( \min_{A \in C} f(A) \). For example, if \( V \) is a set of pixels in an image, one might wish to choose a subset of pixels corresponding to a particular object over which the properties (i.e., color, luminance, texture) are relatively homogeneous. Finding a set \( X \) of size \( k \), even if \( k \) is large, need not have a large valuation \( f(X) \), in fact it could even have the least valuation. Thus, semantic image segmentation could work even if the object being segmented and isolated consists of the majority of image pixels.

As another example, clustering is a problem that often asks for subsets of data that are homogeneous in some way --- one may wish to cluster a dataset \( V \) by removing, one by one, subsets \( X \) from \( V \) that are homogeneous, and this would mean finding a subset with minimum valuation \( f(X) \). As a third example, suppose we are interested in the most probable assignment to a random vector (i.e., MAP probabilistic inference) in the probability model \( p(X) = \frac{1}{Z} \exp(-f(X)) \). Here the function \( f \) is the energy function, \( Z \) is the “partition” function, and \( p(X) \) is said to be a log-supermodular probabilistic model. Log-supermodular models give high probability to configurations of the random variables that are homogeneous or “regular” as measured by \( f \) (since \( f \) gives such configurations a low value). Finding the MAP solution is the same as finding the minimum energy configuration, and if \( f \) is submodular, this is submodular minimization. Probabilistic modeling with submodular/supermodular functions is further discussed in Section 3.5.

Arbitrary set functions are impossible to tractably optimize while having any form of mathematical quality assurance. In fact, it is easy, given a set \( X^* \) with \( |X^*| = k \), to define a function \( f \) such that \( f(X) = \alpha \) for
all $X \neq X^*$ and $f(X^*) = \beta$. With the right values of $\alpha < \beta$, we see that, when trying to maximize this function, anything other than a full exponential (in $n$) search will give an unboundedly large error in the worst case, regardless of the outcome of the $P = NP$ question. Fortunately, this function is not submodular since given sets $Z_1, Z_2$ with $Z_1 \neq Z_2$ and $Z_1 \cup Z_2 = X^*$, we have $f(Z_1) + f(Z_2) = \alpha < \beta + \alpha = f(Z_1 \cup Z_2) + f(Z_1 \cap Z_2)$. Neither is the function supermodular since given some $Z$ with $|Z \setminus X^*| > 0$ and $|X^* \setminus Z| > 0$, we have $f(X^*) + f(Z) = \beta + \alpha > 2\alpha = f(X^* \cup Z) + f(X^* \cap Z)$. Therefore, we might expect there is some hope when we require the function to be submodular.

Submodular optimization problems are more interesting when we impose constraints. For example, when unconstrainedly maximizing a polymatroid function, a trivial solution is $V$ so the problem becomes interesting only when there is a constraint. The simplest and most widely used constraint is the cardinality constraint, giving the following optimization problem: $\text{max}_{X \subseteq V, |X| \leq k} f(X)$. When $f$ represents the information in the set $X$, this optimization procedure asks for the size-limited set $X$ of size $k$ that has the most information about $V$. One way to see this is to note that $f(V) = f(V \setminus X|X) + f(X)$. Thus, when we maximize $f(X)$, we are minimizing the residual information $f(V \setminus X|X)$ about $V$ not contained in $X$.

### 2.3.1 Submodular Maximization

While the cardinality constrained submodular maximization problem is NP complete [Fei98], it was shown in [NWF78; FNW78] that the very simple and efficient greedy algorithm finds an approximate solution guaranteed to be within $1 - 1/e \approx 0.63$ of the optimal solution. Moreover, the approximation ratio achieved by the simple greedy algorithm is provably the best achievable in polynomial time, assuming $P \neq NP$ [Fei98]. The greedy algorithm proceeds as follows: Starting with $X_0 = \emptyset$, we repeat the following greedy step for $i = 0 \ldots (k-1)$:

$$X_{i+1} = X_i \cup \{ \text{argmax } f(X_i \cup \{v\}) \} \quad (25)$$

If there are any ties in the $\text{argmax}$, we break them arbitrarily. What the above approximation result means is that if $X^* \in \text{argmax } \{f(X) : |X| \leq k\}$, and if $\tilde{X}$ is the result of the greedy procedure, then $f(\tilde{X}) \geq (1 - 1/e) f(X^*)$.

It is very easy to show where the famous $1 - 1/e$ approximation ratio comes from, and we show this in the following in as simple and direct a way as possible. From series analysis, we can define $e^x = \lim_{k \to \infty} (1 + x/k)^k$ and since $(1 - 1/k)^k$ is increasing with $k$ having a limit of $e^{-1}$, $1 - (1 - 1/k)^k$ is decreasing with $k$ and has limit of $1 - 1/e$. Then, note that the greedy procedure creates a sequence, or a chain, of elements at step $i$, and we define $X_i = \{v_1, v_2, \ldots, v_i\}$ where $v_i$ is the $i^{th}$ element added by greedy and $X_k$ is the final solution. This forms a chain since $\emptyset = X_0 \subseteq X_1 \subseteq X_2 \subseteq \cdots \subseteq X_i$. Also, with $X^*$ being an optimal set of size $k$ we have

$$f(X^*) \leq f(X^* \cup X_i) = f(X^* | X_i) + f(X_i) \quad (26)$$

$$\leq \sum_{v \in X^*} f(v | X_i) + f(X_i) \quad (27)$$

$$\leq \sum_{v \in X^*} f(v_{i+1} | X_i) + f(X_i) \quad (28)$$

$$= k f(v_{i+1} | X_i) + f(X_i), \quad (29)$$

where Equation (27) follows from submodularity, Equation (28) follows since greedy chooses the optimal single element at each step, and Equation (29) follows since the given optimal solution is one of size $k$. Then

$$f(X^*) - f(X_i) \leq k f(v_{i+1} | X_i) \quad (30)$$

$$= k \left[ f(X_{i+1}) - f(X_i) \right] \quad (31)$$

$$= k \left[ f(X^*) - f(X_i) - \left[ f(X^*) - f(X_{i+1}) \right] \right] \quad (32)$$

which immediately yields

$$f(X^*) - f(X_{i+1}) \leq (1 - 1/k) \left[ f(X^*) - f(X_i) \right] \quad (33)$$

When we note that $f(X_0) = 0$, apply this $k$ times, and use the above bound on $1 - 1/e$, we get

$$f(X^*)(1 - 1/e) \leq f(X^*)(1 - (1 - 1/k)^k) \leq f(X_k). \quad (34)$$
This means that when \( k \) is one, the greedy procedure has an approximation ratio of 1, which is clear since greedy selects the best single element. As \( k \) increases, the approximation ratio gets worse, but it is never worse than the lower bound of \( 1 - 1/e \), but it does mean that the smaller the \( k \) the better the approximation ratio.

The \( 1 - 1/e \) guarantee is a powerful constant factor approximation result since it holds regardless of the size of the initial set \( V \) and regardless of which polymatroid function \( f \) is being optimized. It is possible to make this algorithm run extremely fast using various acceleration tricks [FNW78; NWF78; Min78].

A dual variant for which the greedy algorithm immediately applies is the submodular set cover problem, where one wishes for the smallest set of a given valuation rather than the highest valuation set of a given size. Here we wish to find

\[
X^* \in \text{argmin}_{X \subseteq V} |X| \text{ such that } f(X) \geq a
\]  

(35)

where \( a \) is a minimum valuation threshold. To approximately solve this problem, the greedy algorithm above runs until \( f(X_i) \geq a \) and \( X_i \) becomes the solution. Observe that we then get a solution that satisfies the given constraint (since that is what determines the stopping point). The approximation is in terms of how much bigger the resulting set is than \( |X^*| \). For a general real-valued polymatroid function, the size of the greedy solution \( \tilde{X} = X_i \) that first exceeds the threshold satisfies the following upper bound:

\[
|\tilde{X}| \leq |X^*| \left( 1 + \ln \frac{f(V)}{f(V) - f(\emptyset)} \right) \]

[Wol82]. It is interesting to note that these approximations are the best approximations we can do for these problems in polynomial time, assuming \( P \neq \text{NP} \).

A minor bit of additional information about a polymatroid function, however, can improve the approximation guarantee. Define the total curvature if the polymatroid function \( f \) as

\[
\kappa = 1 - \min_{u \in V} f(v|V - v)/f(v)
\]

where we assume \( f(v) > 0 \) for all \( v \) (if not, we may prune them from the ground set since such elements can never improve a polymatroid function valuation). We thus have \( 0 \leq \kappa \leq 1 \), and [CC84] showed that the greedy algorithm gives a guarantee of \( \kappa (1 - e^{-\kappa}) \geq 1 - 1/e \). In fact, this is an equality (and we get the same bound) when \( \kappa = 1 \), which is the fully curved case. As \( \kappa \) gets smaller, the bound improves, until we reach the \( \kappa = 0 \) case and the bound becomes unity. Observe that \( \kappa = 0 \) if and only if the function is modular, in which case the greedy algorithm is optimal for the cardinality constrained maximization problem. Extending this even further, in many cases, the function need not even be submodular for the greedy algorithm to have a guarantee. Given a non-negative but otherwise arbitrary set function \( h \), the submodularity ratio [DK18] can be defined as a measure of deviation from submodularity as follows:

\[
\gamma(h) = \min_{X \subseteq Y \subseteq V : Y \cap X = \emptyset} \frac{\sum_{v \in Y} h(v|X)}{h(Y|X)}
\]

(36)

where \( |V| = n \). \( h \) is submodular if and only \( \gamma(h) = 1 \), and otherwise \( \gamma(h) < 1 \) measures how far, in a sense, \( h \) is from being submodular. Moreover, a variety of non-submodular functions can be optimized approximately with guarantees that are a function of \( \gamma(h) \). Unfortunately, \( \gamma(h) \) is in general information theoretically hard to compute. In some cases, non-submodular functions can be decomposed into components that each might be more amenable to approximation. We see below that any set function can be written as a difference of submodular [NB05; IB12] functions, and sometimes (but not always) a given \( h \) can be composed into a monotone submodular plus a monotone supermodular function, or a BP function [BB18], i.e., \( h = f + g \) where \( f \) is submodular and \( g \) is supermodular. \( g \) has an easily computed quantity called the supermodular curvature \( \kappa^g = 1 - \min_{v \in V} g(v)/g(v|V - v) \) that, together with the submodular curvature, can be used to produce an approximation ratio having the form \( \frac{\kappa^g}{\kappa^g (1 - e^{-\kappa^g (1-\kappa)})} \) for greedily maximization of \( h \).

In sum, while the greedy algorithm for cardinality constrained maximization might seem overly simple, it is actually quite powerful and computationally unimprovable in the case of polymatroid functions.

### 2.3.2 Discrete Constraints

There are many other types of constraints one might desire besides a cardinality limitation. The next simplest constraint allows each element \( v \) to have a non-negative cost, say \( m(v) \in \mathbb{R}_+ \). In fact, this means that the costs are modular, i.e., the cost of any set \( X \) is \( m(X) = \sum_{v \in X} m(v) \). A submodular maximization problem subject to a knapsack constraint then takes the form \( \max_{X \subseteq V : m(X) \leq b} f(X) \) where \( b \) is a non-negative budget.
While the greedy algorithm does not solve this problem directly, a slightly modified cost-scaled version of the greedy algorithm [Svi04] does solve this problem for any set of knapsack costs. This has been used for various multi-document summarization tasks [LB11; LB12].

When performing convex minimization, a natural constraint to use is a convex subset of the reals. There is no single direct analogy for a convex set when one is optimizing over subsets of the set \( V \), but there are a few forms of discrete constraints that are both mathematically interesting and that often occur repeatedly in applications.

The first form is the independent subsets of a matroid. Firstly, matroids is an area in discrete mathematics that, to do them justice, would require an entire book [Oxl11]. Secondly, to really understand submodularity, one must also master matroids, and this can take some time. For the purposes of this section, we give only the briefest of introductions to matroids, enough to see how they can be useful for constraints in submodular maximization problems. A matroid is an algebraic set system that consists of a set \( V \) and a set of subsets \( I = (I_1, I_2, \ldots) \) known as the independent sets of a matroid, where \( I_i \subseteq V \) for all \( i \). A matroid can fully defined this way and is often indicated by the pair \((V, I)\). To be a matroid, the set of sets must have certain properties, namely: (1) \( \emptyset \in I \); (2) If \( Y \in I \) and \( X \subseteq Y \), then \( X \in I \); and (3) If \( X, Y \in I \) with \( |X| < |Y| \), then \( \exists v \in Y \setminus X \) such that \( Y + v \in I \). The first property says that the set of sets is not empty and must contain the empty set at the very least. The second property says that the set of sets are closed under subsets. The third property is a form of exchangeability, meaning that if we have two independent sets, one larger than the other, there must be an element in the larger independent set that can be added to the smaller independent set without loss of independence. You would not be wrong if the set of independent sets reminds you of sets of independent vectors in a vector space --- in fact, matroids are a purely algebraic generalization of linear independence properties of sets of vectors. Importantly, it is a strict generalization, meaning that there are matroids that are not representable as independent vectors in a vector space over any field [Oxl11].

The independent sets of a matroid are useful to represent a constraint set for submodular maximization [Cal+07; LSV09; Lee+10], \( \max_{X \in I} f(X) \), and this can be useful in many ways. We can see this by showing a simple example of what is known as a partition matroid. Consider a partition \( V = \{ V_1, V_2, \ldots, V_m \} \) of \( V \) into \( m \) mutually disjoint subsets that we call blocks. Suppose also that for each of the \( m \) blocks, there is a positive integer limit \( \ell_i \) for \( i \in [m] \). Consider next the set of sets formed by taking all subsets of \( V \) such that each subset has intersection with \( V_i \) no more than \( \ell_i \) for each \( i \). I.e., consider

\[
I_p = \{ X : \forall i \in [m], |V_i \cap X| \leq \ell_i \}.
\]

Then \((V, I_p)\) is a matroid. The corresponding submodular maximization problem is a natural generalization of the cardinality constraint in that, rather than having a fixed number of elements beyond which we are uninterested, the set of elements \( V \) is organized into groups, and here we have a fixed per-group limit beyond which we are uninterested. This is useful for fairness applications since the solution must be distributed over the blocks of the matroid. Still, there are many much more powerful types of matroids that one can use [Oxl11; GM12].

Regardless of the matroid, the problem \( \max_{X \in I} f(X) \) can be solved, with a 1/2 approximation factor, using the same greedy algorithm as above [NWF78; FNW78]. Indeed, the greedy algorithm has an intimate relationship with submodularity, a fact that is well studied in some of the seminal works on submodularity [Edm70; Lov83; Sch04]. It is also possible to define constraints consisting of an intersection of matroids, meaning that the solution must be simultaneously independent in multiple distinct matroids. Adding on to this, we might wish a set to be independent in multiple matroids and also satisfy a knapsack constraint. Knapsack constraints are not matroid constraints, since there can be multiple maximal cost solutions that are not the same size (as must be the case in a matroid). It is also possible to define discrete constraints using level sets of another completely different submodular function [IB13] --- given two submodular functions \( f \) and \( g \), this leads to optimization problems of the form \( \max_{X \subseteq V : g(X) \leq \alpha} f(X) \) (the submodular cost submodular knapsack, or SCSK, problem) and \( \min_{X \subseteq V : g(X) \geq \alpha} f(X) \) (the submodular cost submodular cover, or SCSC, problem). Other examples include covering constraints [IN09], and cut constraints [JB16]. Indeed, the type of constraints on submodular maximization for which good and scalable algorithms exist is quite vast, and still growing.

One last note on submodular maximization. In the above, the function \( f \) has been assumed to be a polymatroid function. There are many submodular functions that are not monotone [Buc+12]. One example we saw before, namely the graph cut function. Another example is the log of the determinant
(log-determinant) of a submatrix of a positive-definite matrix (which is the Gaussian entropy plus a constant). Suppose that $M$ is an $n \times n$ symmetric positive-definite (SPD) matrix, and that $M_X$ is a row-column submatrix (i.e., it is an $|X| \times |X|$ matrix consisting of the rows and columns of $M$ consisting of the elements in $X$). Then the function defined as $f(X) = \log \det(M_X)$ is submodular but not necessarily monotone non-decreasing. In fact, the submodularity of the log-determinant function is one of the reasons that determinantal point processes (DPPs), which instantiate probability distributions over sets in such a way that high probability is given to those subsets that are diverse according to $M$, are useful for certain tasks where we wish to probabilistically model diversity [KT11]. Diversity of a set $X$ here is measured by the volume of the parallelepiped which is known to be computed as the determinant of the submatrix $M_X$ and taking the log of this volume makes the function submodular in $X$. A DPP in fact is an example of a log-submodular probabilistic model (more in Section 3.5). Also, a relatively simple randomized greedy algorithm [Buc+12] can yield a 1/2 approximation algorithm for maximizing any non-monotone submodular function, a class that includes not only DPPs but also graph cuts and differences between a submodular and a modular function. Interestingly, the log-determinant can be seen as a function of spectral decompositions of principle submatrices of a given SPD matrix, but it is not the only one that is submodular [FG11].

### 2.3.3 Submodular Function Minimization

So far, we have spoken mostly about submodular maximization, but submodular minimization is also a fascinating study, perhaps even more so than submodular maximization. We discussed, for example, the MAP inference problem (amongst others) above.

In the case of a polymatroid function, unconstrained minimization is again trivial. However, even in the unconstrained case, the minimization of an arbitrary (i.e., not necessarily monotone) submodular function $\min_{X \subseteq V} f(X)$ might seem hopelessly intractable. Unconstrained submodular maximization is NP-hard (albeit approximable), and this is not surprising given that there are an exponential number of sets needing to be considered. Remarkably, submodular minimization does not require exponential computation, is not NP-hard, and in fact, there are polynomial time algorithms for doing so, something that is not at all obvious. This is one of the important characteristics that submodular functions share with convex functions, their common amenability to minimization. Starting in the very late 1960s and spearheaded by individuals such as Jack Edmonds [Edm70], there was a concerted effort in the discrete mathematics community in search of either an algorithm that could minimize a submodular function in polynomial time or a proof that such a problem was NP-hard. The nut was finally cracked in a classic paper [GLS81] on the ellipsoid algorithm that gave a polynomial time algorithm for submodular function minimization (SFM). While the algorithm was polynomial, it was a continuous algorithm, and it was not practical, so the search continued for a purely combinatorial strongly polynomial time algorithm. Queyranne [Que98] then proved that an algorithm [N92] worked for this problem when the set function also satisfies a symmetry condition (i.e., $\forall X \subseteq V, f(X) = f(V \setminus X)$), which only requires $O(n^5)$ time. The result finally came around the year 2000 using two mostly independent methods [IFF00; Sch00]. These algorithms, however, also were impractical in that while they are polynomial time, they have unrealistically high polynomial degree (i.e., $\tilde{O}(V^{7}\gamma + V^8 \gamma)$ for [Sch00] and $\tilde{O}(V^{7}\gamma)$ for [IFF00]). This led to additional work on combinatorial algorithms for SFM leading to algorithms that could perform SFM in time $\tilde{O}(V^{5}\gamma + V^6 \gamma)$ in [IO09]. Two practical algorithms for SFM include the Fujishige-Wolfe procedure [Fuj05; Wol76] as well as the Frank-Wolfe procedure, each of which minimize the 2-norm on a polyhedron $B_f$ associated with the submodular function $f$ and which is defined below (it should also be noted that the Frank-Wolfe algorithm can also be used to minimize the convex extension of the function, something that is relatively easy to compute via the Lovász extension [Lov83], see below). More recent work on SFM are also based continuous relaxations of the problem in some form or another, leading algorithms with strongly polynomial running time [LSW15] of $O(n^3 \log^2 n)$ for which it was possible to drop the log factors leading to a complexity of $O(n^3)$ in [Jia21], weakly-polynomial running time [LSW15] of $\tilde{O}(n^2 \log M)$ (where $M = \max_{S \subseteq V} |f(S)|$), pseudo-polynomial running time [ALS20; Cha+17] of $\tilde{O}(nM^2)$, and a $\epsilon$-approximate minimization with a linear running time [ALS20] of $\tilde{O}(n/\epsilon^2)$. There have been other efforts to utilize parallelism to further improve SFM [BS20].

What is remarkable about all of the above algorithms is that while submodular functions live in a cone in

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$^3$ This is the same Wolfe as the Wolfe in Frank-Wolfe but not the same algorithm.
2ⁿ-dimensional space, this cone has a non-empty (measurable) interior. This means that it is not possible to map this cone of points down to a lower-dimensional space, or equivalently, that submodular functions in general have 2ⁿ independent degrees of freedom (at least locally). This can be seen by considering strictly submodular functions, ones for which the inequality is never an equality, even such simple functions like \( \sqrt{|X|} \). Even in such rich a space, submodular functions can be minimized with so few oracle queries to \( f \).

The above polytime (and in particular the \( \tilde{O}(n/e^2) \)) results are particular interesting. As \( n \to \infty \) the ratio of points that are queried to minimize a submodular function, and independent points the submodular function contains, goes to zero. This is quite analogous to convex functions.

Practically speaking, with so many algorithms capable of minimizing a submodular function, it may not be obvious which one to choose. In general, the practical utility of the various algorithms, even the ones with lower asymptotic complexity, have not been compared to the Fujishige-Wolfe and Frank-Wolfe procedures (which are the ones used most often in practice for general purpose submodular function minimization). If the submodular function is a special case, however (e.g., the graph cut function) then it is in general better to use an algorithm specifically geared towards exploiting the additional extant structure. Also, sometimes the minimum norm can be slow, and even though SFM is polytime, it is sometimes useful to approximately minimize a submodular function [JLB11].

### 2.3.4 Other Submodular Optimization Problems

Besides maximization and minimization, there are other discrete optimization problems involving submodular that are interesting and useful. In this section, we consider several of them.

Firstly, the above submodular greedy maximization procedure has a guarantee only if the function is submodular and monotone non-decreasing. A simple trick can be used to find a solution when the function is monotone non-increasing. Suppose that \( f \) is submodular and monotone non-increasing, so that \( f(X) \geq f(Y) \) whenever \( X \supseteq Y \). We define a function \( g \) so that \( g(X) = f(V \setminus X) \), so now, whenever \( X \supseteq Y \), \( g(X) = f(V \setminus X) \leq f(V \setminus Y) = g(Y) \) and hence \( g \) is monotone non-decreasing and is also submodular. Using the greedy algorithm, or whatever procedure we wish, let \( \tilde{X} \) be a set of size \( k \) having \( g(\tilde{X}) \geq g(X') \) where \( X' \in \text{argmax}_{X \subseteq V : |X| \leq k} g(X) \). Thus, \( f(\tilde{V} \setminus \tilde{X}) \geq af(V \setminus \tilde{X}) \) for all \( X \subseteq V \) with \( |X| = k \). Thus, we’ve found a set \( \tilde{Z} = V \setminus \tilde{X} \) of size \( k' = n - k \) such that \( f(\tilde{Z}) \geq af(Z) \) for any set \( Z \) of size \( k' \).

Often, however, the submodular function is itself neither monotone non-decreasing nor monotone non-increasing, e.g., the graph cut or the log-determinant functions. In such cases, there are both randomized and deterministic algorithms [Buc+12; BF18] some of which are quite simple. For example, the bidirectional greedy algorithm of [Buc+12] takes elements in a random order, and randomly inserts the element into either a growing set or removes the element from a shrinking set depending on probabilities based on the gain change. These algorithms give a \( O(1/2) \) guarantee for unconstrained non-monotone submodular maximization, which is the best one can do in polynomial time.

In some cases, submodular maximization alone does not suffice, and we wish for the solution to be robust to deletions. For example, in summarization problems (see Section 3.1), once a summary has been constructed, a deletion request might be made on a certain number of elements in the summary. We may therefore wish to ensure that the remaining summary after deletion is still highly valued by the submodular function. This idea leads to an optimization problem [OSU18] of the form:

\[
\max_{X \subseteq V : |X| \leq k} \min_{Y \subseteq X : |Y| \leq k'} f(X \setminus Y) \quad (38)
\]

Here we wish to maximize the submodular function under a cardinality constraint of size \( k \) but in such a way that the solution is robust even to the worst-case deletion of a set of size \( k' \). For any set \( Y \subseteq X \), the function \( f_Y(X) = f(X \setminus Y) \) is submodular in \( X \) and thus the above optimization problem can be expressed as the maximization of the minimum over of a set of submodular functions [Kra+08].

\[
\max_{X \subseteq V : |X| \leq k} \min_{i} f_i(X) \quad (39)
\]

Seeing the problem this way is not without a loss of useful structure that is exploited in [OSU18], but if the inner minimization is over only a relatively small number of submodular functions, then a bi-criterion guarantee can be obtained using a binary search procedure [Kra+08; Pow+16; Cot+18].
As mentioned elsewhere, clustering is the problem of grouping items together that are homogeneous in some way. A submodular function, when maximized, prefers heterogeneous items and when minimized prefers homogeneous items. Using these notions, there are ways to use submodular objectives to determine such properties in a way that is very flexible, as flexible as the space of submodular functions. The general approach is to partition the set $V$ into blocks. Here, the submodular function itself is used to construct the partition, unlike with a partition matroid (above) where the partition is pre-constructed and used as a constraint. The most general form of problems takes the following forms:

\[
\text{Diverse Blocks Partitioning Problem: } \max_{\pi \in \Pi_m} \left[ \bar{\lambda} \min_i f_i(X_i^n) + \frac{\lambda}{m} \sum_{j=1}^{m} f_j(X_j^n) \right], \tag{40}
\]

\[
\text{Homogeneous Block Partitioning Problem: } \min_{\pi \in \Pi_m} \left[ \bar{\lambda} \max_i f_i(X_i^n) + \frac{\lambda}{m} \sum_{j=1}^{m} f_j(X_j^n) \right]. \tag{41}
\]

where $0 \leq \lambda \leq 1$, is a tradeoff parameter, $\bar{\lambda} = 1 - \lambda$ is the complement of the tradeoff parameter, the set of sets $\pi = (X_1^n, X_2^n, \cdots, X_m^n)$ is a partition of the ground set $V$ (i.e., recall from above, $\cup_i X_i^n = V$ and $\forall i \neq j, X_i^n \cap X_j^n = \emptyset$), and $\Pi_m$ refers to the set of all possible partitions of $V$ into $m$ blocks. The parameter $\lambda$ controls the objective: $\lambda = 1$ is the average case, $\lambda = 0$ is the robust case, and $0 < \lambda < 1$ is a mixed case. In general, these problems are intractable even to approximate. Assuming $f_1, f_2, \cdots, f_m$ are all polymatroid functions, however, enables relatively simple algorithms to have approximation guarantees. Polymatroid functions also mean that the partitioning problems are natural to a variety of practical problems. Often it is assumed that the $f_i$’s are identical to each other (the homogeneous case) as the problem becomes similar, while the more general heterogeneous case is stated above. Taken together, these problems are called Submodular Partitioning.

Problem 40 asks for a partition whose blocks each (and that collectively) have a high valuation according to the polymatroid functions. Problem 40 with $\lambda = 0$ is called submodular fair allocation (SFA), where the goal is to choose the partition so that the worse valued block is as large as possible. If one thinks of $V$ as consumable goods that can be allocated to people, and $f_i$ as a valuation function for person $i$, this problem ensures that the poorest person gets well taken care of. Problem 40 for $\lambda = 1$, on the other hand, is called submodular welfare. Again, when $V$ is a set of goods, this procedure asks only that the average allocation of goods to consumers is high, even if the partition allocates little to the poorest and much to the richest individual. For various additional assumptions on the submodular functions, there is much to exploit. For the $\lambda = 0$ case, see [AS10; Gol05; KP07], while for the $\lambda = 1$ case, see [Von08; FNW78; Von08].

Problem 41 asks for a partition whose blocks each (and that collectively) are internally homogeneous. This is typically the goal in clustering algorithms so we can think of problem 41 as a submodular generalization of clustering. When $\lambda = 0$, Problem 41 is called the submodular load balancing (SLB) problem and when $f_i$’s are all modular, it is called minimum makespan scheduling. Like above, are solutions for such special cases [HS88; LST90]. Even in the homogeneous submodular case, however, the problem is shows that the problem [SF08] is information theoretically hard to approximate within $o(\sqrt{n/\log n})$. When $\lambda = 1$, problem 41 becomes the submodular multiway partition (SMP) problem for which one can obtain $2$-approximations [CE11a; ZNI04; NJB05a] in the homogeneous case and $O(\log n)$ [CE11b] in the heterogeneous case.

The general $0 \leq \lambda \leq 1$ case for both Problem 40 and 41 was addressed in [Wei+15b] and in the Problem 40, this was extended in [Cot+18] to include a submodular cross-block diversity term in the objective, i.e., one that prefers not only intra-block but also inter-block diversity.

Even when the function of interest is not submodular, but is approximately submodular, or decomposable into submodular components, algorithms for submodular optimization can be relied on to behave reasonably well. For example, another form of submodular optimization strives to minimize a non-submodular function that has been decomposed into a difference of submodular functions. Let $h : 2^V \to \mathbb{R}$ be any arbitrary set function, meaning neither submodular nor supermodular nor possessing any other useful structural property. Then there are two polymatroid functions $f$ and $g$ such that we can decompose $h$ into a difference --- this means that for all $X$, $h(X) = f(X) - g(X)$. Very much like the difference of concave (DC) optimization, this is known as a difference of submodular (or DS) decomposition [NB05; IB12] of $h$ and we may, exploiting the properties of this decomposition, either maximize or minimize $h$. This can be particularly useful when
the function \( h \) has a natural decomposition, for example the mutual information function when seen as a set function where \( h(X) = I(R_X; R_Y) = H(R_X) - H(R_X | R_Y) = f(X) - g(X) \). This is a DS decomposition since both \( f(X) = H(R_X) \) and \( g(X) = H(R_X | R_Y) \) are polymatroid functions in \( X \). In fact, submodular functions can be used to define generalized combinatorial forms of mutual and conditional mutual information [Iye+21b], ones that are much more practical for a variety of problems since even computing one entropic query can involve a complex probabilistic inference problem. A special case of DS optimization asks to maximize the sum of a monotone submodular and a monotone supermodular (or a BP) function and this was studied in [BB18] (more on this below).

Algorithms for DS and BP optimization use a form of discrete semi-gradients, analogous to semi-gradients that exists for concave and convex functions, except for here there are sub-gradient and super-gradients that are available both for submodular and supermodular functions. This is another reason that submodular functions are both like and unlike both convex and concave functions. Related to DS problems are those that involve maximizing one submodular objective while using another submodular objective as a constraint, which use the second function to define submodular sublevel sets in problems such as \( \max_{X} f(X) \) subject to \( g(X) \leq a \) or alternatively, \( \min_{X} f(X) \) subject to \( g(X) \geq a \), as was introduced in [IB13]. Instances of using multiple submodular functions in this way, and comparing DS and constrained optimization formulations, was explored for speech recognition applications in [Liu+17].

### 2.4 Continuity, Polyhedra, and Extensions

One of the strategies for optimizing submodular functions is via continuous relaxations. On this topic, another way that submodular functions are like convex functions, and that is related to their continuous extension. Recall from above that a submodular function is defined by offering a value to every vertex of the \( n \)-dimensional hypercube.

Recall, any continuous valued function can be transformed into a unique convex function via its convex envelope. That is, given any function \( h : D_h \to \mathbb{R} \), where \( D_h \subseteq \mathbb{R}^n \), we may define a new function \( \hat{h} : \mathbb{R}^n \to \mathbb{R} \) via the following

\[
\hat{h}(x) = \sup\{g(x) : g \text{ is convex } \& \ g(y) \leq h(y), \forall y \in D_h\}.
\]

(42)

It can be shown that (1) \( \hat{h}(x) \) is convex, (2) \( \hat{h}(x) \leq h(x), \forall x \), and (3) if \( g(x) \) is any convex function having the property that \( g(x) \leq h(x), \forall x \), then \( g(x) \leq \hat{h}(x) \). The function \( \hat{h}(x) \) is the convex envelope of \( h \), and is in some sense the everywhere-largest-valued function lower than \( h \) that is still convex.

Submodular functions are discrete functions, so in order to extend them to a continuous function, and then compute the convex envelope, we must start by placing the value \( f(X) \) for each \( X \) at some coordinate in continuous space, and for this purpose we use the vertices of the hypercube. A continuous extension \( \tilde{f} : \mathbb{R}^V \to \mathbb{R} \) of a set function \( f : 2^V \to \mathbb{R} \) is a continuous function that agrees with the set function on all vertices of the hypercube. This means that \( \tilde{f}(1_X) = f(X) \) for all \( X \subseteq V \). Any set function has an infinite number of continuous extensions, and any set function has an infinite number of extensions that may be either convex or concave. The tightest convex extension of an arbitrary set function is known as the convex closure, which is a function \( \hat{f}(x) : [0, 1]^V \to \mathbb{R} \) defined in the following way:

\[
\hat{f}(x) = \min_{p \in \Delta^n(x)} \sum_{X \subseteq V} p_X f(X)
\]

(43)

where \( \Delta^n(x) = \{p \in \mathbb{R}^2^n : \sum_{X \subseteq V} p_X = 1; \ p_X \geq 0, \ \forall X \subseteq V; \ & \sum_{X \subseteq V} p_X 1_X = x\} \) is the probability simplex in \( 2^n \) dimensions. It can be shown that \( \hat{f}(x) \) tight (i.e., \( \forall X \subseteq V \), we have \( \hat{f}(1_X) = f(X) \)), that \( \hat{f} \) is convex (and thus, that any arbitrary set function has a tight convex extension), that the convex closure \( \hat{f} \) is the convex envelope of a function taking values only on the hypercube vertices, and which takes value \( f(X) \) on hypercube vertex \( 1_X \) for all \( X \subseteq V \).

We say it is tightest such convex continuous extension of \( f \) in the sense that it is the convex envelope. It is also apparent that the function is defined as a minimization over an exponentially large (in \( n \)) space of a sum over an exponential number of terms. Some immediate and interesting questions, then, to ask are: (1) when
is \( \tilde{f}(x) \) computationally feasible to obtain or estimate? (2) When does \( \tilde{f}(x) \) have interesting mathematical properties? and (3) When is \( \tilde{f}(x) \) useful as a surrogate for a given \( f \)? It turns out that when \( f \) is submodular, there will be good answers to all three questions as we shall now see.

The first quantity we will need to define is the submodular polyhedron, i.e., the polyhedron \( \mathcal{P}_f \) associated with a submodular function \( f \).

\[
\mathcal{P}_f = \{ x \in \mathbb{R}^V : x(A) \leq f(A), \forall A \subseteq V \} \tag{44}
\]

This polyhedron lies within an \(|V|\)-dimensional space and is defined via an exponential set of inequalities. It can be shown that this polyhedron contains the same information as \( f \) (i.e., given \( \mathcal{P}_f \) we can reconstruct \( f \)). When \( f \) is a polymatroid function, then \( \mathcal{P}_f \cap \mathbb{R}_+ \) is called a polymatroid since, for a variety of reasons, it is a natural polyhedral generalization of a matroid. It is for this reason that non-negative monotone non-decreasing submodular functions are called polymatroid functions as we mentioned above.

We also define a polytope associated with a submodular function called the base polytope defined as

\[
\mathcal{B}_f = \mathcal{P}_f \cap \{ x \in \mathbb{R}^V : x(V) = f(V) \} \tag{45}
\]

Since \( \mathcal{B}_f \) can also have an exponential (in \( n \)) number of facets, we would expect that using \( \mathcal{B}_f \) as a constraint in a linear programming problem would lead to an intractability. Indeed, consider the following parameterized linear programming problem which defines a function \( \tilde{f} : \mathbb{R}^V \to \mathbb{R} \):

\[
\tilde{f}(x) = \max(x^\top y : y \in \mathcal{B}_f). \tag{46}
\]

This function is convex (since it maximizes over a set of linear functions) but interestingly, when \( f \) is submodular, we have that \( \tilde{f}(x) = \tilde{f}(x) \). Even more interestingly, \( \tilde{f} \) is possible to compute this function easily using what is known as the Lovász extension, defined as follows. Given a particular \( x \), find an ordering \( \sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n) \) of the elements in \( V \) where \( \sigma_i \in [V] \) that sorts the elements of \( x \) descending, meaning that \( x_{\sigma_1} \geq x_{\sigma_2} \geq \cdots \geq x_{\sigma_n} \). We also define a series of sets \( S_i = \{ \sigma_1, \sigma_2, \ldots, \sigma_i \} \) for \( i \in [n] \); thus \( \emptyset = S_0 \subseteq S_1 \subseteq S_2 \subseteq \cdots \subseteq S_n = V \). Such a sequence of sets is called a chain. Then Lovász [Lov83] showed that

\[
\tilde{f}(x) = x_{\sigma_n} f(V) + \sum_{i=1}^{n-1} (x_{\sigma_i} - x_{\sigma_{i+1}}) f(S_i) = \sum_{i=1}^{n} \lambda_i f(S_i) \tag{47}
\]

where \( \lambda_i \) is defined accordingly. We see that computing this expression is relatively easy --- it requires only a sort of the elements of \( x \) and then \( O(n) \) evaluations of \( \tilde{f} \), much better than the exponential costs seen above.

The right-hand side of Equation (47), in and of itself, by no means is guaranteed to be convex. Lovász [Lov83] showed, however, that not only is this expression equal to the convex closure of the submodular function, but that the expression on the right of Equation (47) is convex if and only if \( f \) is submodular. This is a strong relationship between submodular and convex functions and is one of the reasons it was possible to show that submodular function minimization was possible in polynomial time [GLS81] as mentioned earlier. One should also be aware that the Lovász extension is equivalent to the Choquet integral [Cho53] which was defined much earlier.

On the other hand, fondly recall the simple example of submodular function \( f(X) = \sqrt{|X|} \) or the feature-based submodular functions \( f(A) = \sum_{u \in U} \phi_u(\sum_{a \in A} m_{u,a}) \) where \( \phi_u \) are concave. So, while the convex closure of a submodular function is easy to compute, and the form of the extension is convex if and only if the function \( f \) is submodular, it is a concave (not a convex) function composed with a modular function that is submodular. Thus, asking if a submodular function is more concave-like or more convex-like, or neither, is really a meaningless question. Indeed, it is important to realize that submodularity defines inequalities between variables of different dimensions, while convexity also requires a certain relationship even amongst values in the same dimension and is convex in all directions (e.g., if \( \psi : \mathbb{R}^n \to \mathbb{R} \) is a convex function and we define \( \tilde{\psi}(x,y) = \psi(x + ay) \), then \( \tilde{\psi} : \mathbb{R} \to \mathbb{R} \) is also convex). There is no such corresponding operation possible with submodular functions, although there are analogous argument restrictions for set functions that preserve submodularity (these include subset restrictions, as we saw above).

Speaking of concave composed with modular functions, recall that \( \phi(m(X)) \) is submodular whenever \( \phi : \mathbb{R} \to \mathbb{R} \) is concave. Supposing instead that \( \phi : \mathbb{R}^V \to \mathbb{R} \) is a multivariate real-valued function, and then
we construct set function as via \( f(X) = \phi(1_X) \). We can easily see, by considering multivariate quadratic functions, that concavity of \( \phi \) is insufficient to ensure the submodularity of \( f(X) \). Consider a concave \( \phi : \mathbb{R}^2 \rightarrow \mathbb{R} \) defined as \( \phi(x) = x^T M x \) where \( M = \begin{pmatrix} -2 & -1 \\ -1 & -1 \end{pmatrix} \). This matrix has negative eigenvalues, and thus \( \phi \) is concave, but we see that \( \phi(1_X) + \phi(1_Y) = -3 - 2 < -3 + 0 = \phi(1_{X \cup Y}) + \phi(1_{X \cap Y}) \) when \( 1_X = \left( \frac{1}{1} \right) \) and \( 1_Y = \left( \frac{1}{1} \right) \).

There is, however, another condition on a multivariate real-valued function that is sufficient to ensure submodularity and that also is useful in its own right, and that is based on a continuous form of submodularity. We can define a form of continuous submodularity on real-valued vectors as follows. Given two real-valued vectors \( x, y \) the submodularity of a function \( \phi : \mathbb{R}^n \rightarrow \mathbb{R} \) is defined as:

\[
\phi(x) + \phi(y) \geq \phi(x \lor y) + \phi(x \land y)
\]

where the join \( x \lor y \) is defined as the vector with the element-wise maximums of the two (i.e., \( (x \lor y)(i) = \max(x(i), y(i)) \)) and \( x \land y \) is the vector of element-wise minimums. We see this definition coincides with the standard discrete definition of submodularity (Definition 2.1) whenever \( x, y \in \{0, 1\}^n \) are characteristic vectors of sets. If \( \phi \) is also differentiable, this definition is identical to the Hessian matrix of \( \phi \) having non-positive off-diagonal entries. That is, for all \( x \), we have that

\[
\forall i \neq j, \quad \frac{\partial^2 \phi(x)}{\partial x_i \partial x_j} \leq 0
\]

This is analogous to the definition given for supermodularity in the economics literature [Top98; Sam47]. It is important to realize that the above does not place constraints on the diagonal entries of the Hessian. Submodularity in the differentiable case, in general, does not require negatives (or positives) along the diagonal. Therefore, a real valued submodular function might neither be convex nor concave. A simple example of a two-dimensional quadratic would put \( M = \begin{pmatrix} -1 & -2 \\ -2 & -1 \end{pmatrix} \). Here, all the off-diagonal entries are non-positive, and hence the quadratic is submodular, but the quadratic is neither convex nor concave since it has both a positive \((3)\) and a negative \((-1)\) eigenvalue.

For classic discrete submodular functions, there is an equivalent definition of submodularity based on diminishing returns (Definition 2.2). There is also a diminishing returns property in the continuous world as well. This is as follows: for all \( x \leq y \) (taken element-wise, meaning that \( \forall i, x(i) \leq y(i) \)), for all \( v \in V \), for all \( a \geq 0 \), we have \( \phi(x + a1_{\{v\}}) - \phi(x) \geq \phi(y + a1_{\{v\}}) - \phi(y) \). Any real-valued function that satisfies the above is called DR Submodular (for diminishing returns submodular), and it means that any time we have an increment in the positive direction, the increment becomes less valuable if we start from more in the positive direction along any dimension.

For discrete set functions (i.e., functions defined only on vertices of the hypercube), the two definitions, continuous submodularity and DR submodularity, are mathematically identical. In the general continuous case, however, we only have that DR submodularity implies submodularity, but not vice versa (meaning there are submodular functions that are not DR submodular). As an example, consider the quadratic function above with \( M = \begin{pmatrix} 1 & -2 \\ -2 & 1 \end{pmatrix} \). We saw above that such a quadratic is submodular, but it is not DR submodular. If we take a submodular function, however, and also insist that it is coordinate wise concave, then it is DR submodular. Indeed, when differentiable, the DR submodular condition is identical to \( \forall i, j, \frac{\partial^2 \phi(x)}{\partial x_i \partial x_j} \leq 0 \), note that this says for all \( i, j \), not just \( i \neq j \) as in the case of a submodular function. This therefore means that the Hessian matrix is all non-positive, a condition that does not require concavity which requires a non-positive definite Hessian.

When are submodular and DR submodular functions useful? Like the more typical discrete submodular functions, such continuous submodular functions can often be optimized even though they are neither concave nor convex [Bac19; MHK20]. For example, DR submodular functions, despite not being convex, can be exactly minimized [Bia+17] and approximately maximized [BBK19], very much like discrete submodular functions. Also, the deep submodular functions (DSFs) [BB17] mentioned above are often instantiated using certain classes of nested DR-submodular functions. There are also interesting strategies for approximate continuous DR-Submodular maximization [SF20]. Therefore, it seems reasonable that this is a natural generalization of the discrete to the continuous.

Another extension of discrete submodular functions is that of bisubmodularity [CK88; Qi89; Bou+95; AFN96; TF07; MF10; SGB12] and multivariate submodularity [SS19]. A bisubmodular function is of the
form: \( f : 2^V \times 2^V \to \mathbb{R} \). There are several types of bisubmodular functions [Qi89], the common type having the property that \( f(A, B) + f(C, D) \geq f(A \cap C, B \cap D) + f((A \cup C) \setminus (B \cup D), (B \cup D) \setminus (A \cap C)) \) whenever both \( A, B \) and \( C, D \) are nonintersecting. Bisubmodular functions can be seen as a form of signed (or typed) set membership, where an item is a member of a set if it is a member of either \( A \) or \( B \), but the sign is determined by which member. Bisubmodular functions also have polyhedra for which the greedy algorithm can be applied [DW73]. A simpler form of bisubmodularity was defined in [SGB12]. More general still, a submodular function can be defined over any lattice [Bir48; Fan68]. In fact, the submodular and DR submodular functions above defined on real vectors can be considered submodular functions defined on a real lattice, so this is quite general.

### 2.5 Historical Applications of Submodularity

Submodular functions [Fuj05] have a long history in economics [Viv01; Car01; Sam47], game theory [Top98; Sha71], combinatorial optimization [Edm70; Lov83; Sch04], electrical networks [Nar97], and operations research [GGL90]. Entire issues of journals of discrete mathematics have been devoted to their exposition [Sub]. The classic applications of submodularity lie in their use to describe a variety of properties of problems arising in graph theory and combinatorial optimization [Fra93]. The graph cut function mentioned above is one typical example, but there are many others (see [Fra93; Fra98]). Similar to how convergent evolution indicates the utility of a genetic trait, submodularity, under many different names, has been independently discovered in a number of different domains.

For example, in statistical physics, it is sometimes known as the ferromagnetic assumption, standard in the Ising model [Isi25; Pei36] and its generalization to the Potts model [Pot52]. In the Ising case, \( x \in \{0, 1\}^n \) represents a configuration of \( n \) particles and each particle \( x_i \) can be in one of two states \( x_i \in \{-1, +1\} \). Each particle, for example, might be an atom of magnetic material that can have a magnetic moment oriented in either the “up” or the “down” directions. The overall energy of these particles can be described as the Hamiltonian \( \mathcal{E}(x) = -\sum_{(i,j) \in E} \beta x_i x_j \) where \( E \) is the set of edges of a graph. In the ferromagnetic case, \( \beta > 0 \) so that the lowest energy configuration (i.e., \( \sum_{(i,j) \in E} \beta x_i x_j \) is maximum) occurs when all neighboring particles point in the same direction (\( x_i = x_j \)). When used as an energy in a probability model \( P[x] \propto \exp(-\mathcal{E}(x)) \) this lowest energy configuration corresponds to one with the highest probability. How does this correspond to submodularity? Consider any pair \((i, j) \in E\). Since \( \beta > 0 \), we have that \(-\beta \times (-1) \times (+1) - \beta \times (+1) \times (-1) = -\beta \times (+1) \times (+1) - \beta \times (-1) \times (-1) \), but we see that this is precisely the same condition as Equation (48) applied to the Boolean lattice (i.e., 0/1-valued vectors). Moreover, we can see \( \sum_{i \in [n]} x_i \) as a modular function. Hence, minimizing \( \mathcal{E}(x) \) is an instance of submodular function minimization, and the Ising model’s energy function is a special case of a submodular function in the ferromagnetic case.

Another example where submodularity plays a role is in efficiently computing the earth mover’s distance (or Wasserstein metric). We start with a non-negative supply vector \( x = (x_1, x_2, \ldots, x_n) \) (representing the amount or mass of some substance at position \( i \in [n] \)) and demand vector \( y = (y_1, y_2, \ldots, y_m) \) (representing the mass of some substance needed at position \( j \in [m] \)). There is an \( n \times m \) matrix \( C \) where \( C_{ij} \) represents the cost, or distance, to transport a unit of mass between position \( i \) and \( j \). Let \( Z \) be an \( n \times m \) matrix. The goal is to solve the linear programming problem \( \min_Z \sum_{i=1}^n \sum_{j=1}^m C_{ij} Z_{ij} \) subject to \( \sum_{j=1}^m Z_{ij} = x_i \), \( \sum_{i=1}^n Z_{ij} = y_j \), and \( Z_{ij} \geq 0 \). The normalized solution to this problem is the earth mover’s distance. We can view this problem as either a transportation problem (the total mass at locations represented by \( x \) needs to be moved to locations represented by \( y \) in the best possible way) or as a way of computing a best-case distance between two probably mass functions (say if the vectors sum to one). Ordinarily, solving this problem requires general linear programming. Suppose, however, that the costs satisfy the Monge property, i.e.: \( C_{ij} + C_{rs} \leq C_{is} + C_{rj} \) for all \( 1 \leq i < r \leq n \) and \( 1 \leq j < s \leq m \). Then the above transportation problem can then be solved using a simple greedy algorithm (known as the north-west corner rule) in only \( O(n + m) \) time [BKR96]. Now suppose we define a function \( \phi : [n] \times [m] \to \mathbb{R} \) and set \( \phi(i, j) = C_{ij} \). Then \( \phi \) is submodular in the sense of (48) if and only if the matrix \( C \) is Monge. Hence, the submodularity property allows rapid computation of the earth mover’s distance in some cases. This can be generalized to higher dimensional tensors as well [Bei+95] using a form of Monge property that is the same as the multivariate submodularity mentioned in Section 2.4.

We’ve already seen in Section 2.0.3 how the Shannon entropy function is submodular, and how the submodular inequalities are just a restatement of the classic Shannon inequalities [Yeu91; ZY97; ZY98].
block coding applications, we might wish to partition a set of random variables into two disjoint sets so as to minimize the mutual information between them. If we find such a partition, each set of random variables can be block coded with a minimum coding length over all such partitions. If \( S \subseteq V \) is a set of random variables, then minimizing \( f(S) = I(S; V \setminus S) \) (where \( I(\cdot; \cdot) \) is the mutual information function) corresponds precisely to this task. Here, \( f(S) \) is a symmetric submodular function that can be minimized in \( O(n^3) \) time \([Que98; NI92]\) as mentioned in Section 2.3.3. Incidentally, regarding information theory, the von Neumann, or quantum, information \([Neu32]\) also satisfies a property, called “strongly sub-additivity” and considered an essential and fundamental property of quantum information, that is essentially the same as submodularity \([DM36; LR73; RR67]\).

Cooperative game theory is also an area that makes good use of submodularity, or rather supermodularity which of course is quite related. Here, we think of \( V \) as a set of “players”, any subset \( X \subseteq V \) of players is considered a “coalition”, and a function \( f : 2^V \rightarrow \mathbb{R} \) is considered a “game”, in that it assigns a value or worth to each coalition. Interacting players, if they agree, can strategically join a coalition \( X \) and the resulting worth \( f(X) \) must somehow be distributed to the players. As a side note, it is interesting that game theoretic settings were significantly developed and advanced \([VNM44]\) by the same von Neumann who developed quantum information \([Neu32]\) --- besides so many other amazing achievements, he also seems to have touched submodularity in many ways. It is usually the case that games are normalized \( f(\emptyset) = 0 \), superadditive \( f(X) + f(Y) \leq f(X \cup Y) \) so that the joint coalition \( X \cup Y \) is worth no less than the two coalitions acting independently, thereby incentivizing cooperation) and supermodular (Definition 11), although in the game theory literature, supermodularity is sometimes called convex \([Sha71]\) due to the analogy that Definition 11 has with the non-negativity of second derivatives. The way the worth \( f(X) \) is distributed to the players is given by a payoff vector, a normalized modular function \( m \). Those payoff vectors that satisfy both \( m(V) \leq f(V) \) and \( VX \subseteq V \), \( m(X) \geq f(X) \) are those modular functions that aren’t worth more than the entire game, but that would be satisfactory to any coalition. Such payoff vectors are called the core of the game and, collectively, they can be seen as a dual of the base polytope of a submodular function (Equation (45)). The question regarding such a game is what the outcome, or resulting coalition, should be; and also what the right payoff vector is, considering that the core itself can be an infinitely large set. This was addressed in fact by what is known as the Shapley value, which says that the payoff vector should be based on the average contribution of each player to all possible contexts. I.e., the Shapley value \([Sha53]\) is a modular function \( m_{\text{shapley}} \) that can be defined, for all \( v \in V \), as \( m_{\text{shapley}}(v) = \frac{1}{n!} \sum_{\sigma \in \Sigma} f(v_{[\sigma_{<v}]}) \), where \( \Sigma \) is the set of all total orderings of \( V \), \( \sigma \) is a particular ordering, and \( \sigma_{<v} \subseteq V \) is the set of items that precede \( v \) in the order \( \sigma \). While there are other definitions of the Shapley value, this one has an intuitive definition as the average improvement in value that \( v \) provides over all possible coalitions into which \( v \) is added. Hence, this seems to be a reasonable payoff amount for \( v \). Interestingly, the Shapley value is a member of the core of the game. The Shapley value in fact has, of late, become useful as an attribution method \([LL17]\), i.e., to evaluate the contribution of parts of a feature vector for the resulting final output in, for example, a deep neural network.

It is also interesting to note that fuzzy set theory uses fuzzy measures \([GSM00]\) (or capacities) and are a form of non-additive measures \([Pap06]\) on sets in a way that generalizes standard additive (e.g., Lebesque) measures on sets. These measures are often submodular or supermodular functions. Integrals with respect to these non-additive measures can be defined, and one extremely useful one is the Choquet integral \([Cho53]\) which as we have seen earlier is identical to the Lovász extension (Equation (47) and \([Lov83]\)).

In natural language processing, submodularity has been uncovered for a variety of purposes. For example, the popular Rouge-recall metric \([Lin04]\) for judging the quality of a candidate document summary was shown to be submodular \([LB11]\). In statistical machine translation, submodularity also spontaneously arose \([Biç13; KB14]\) for the purposes of selecting a subset of training data that was specifically relative for a given test translation task. In computer vision, Markov random fields were at one time all the rage, and since solving them in general was known to be intractable, there was a concerted effort to identify conditions that enabled their practical and tractable solution. Submodularity arose as that condition, although it was at that time called, or was strongly related to, potential functions which are called “regular”, “Potts”, or “attractive” \([BVZ01a; KZ02; KZ04; BK04; KT08; KK09; JB16]\). Algorithms related to graph cut can often solve such models either exactly or approximately well. This research led to algorithms that overcame pure binary image segmentation and led to move-making algorithms such as alpha expansions and alpha-beta swaps \([BVZ01a; KZ02; BK04]\). This had a big impact on problems such as semantic image segmentation. Since these are based on Markov random fields but with restricted potential functions, submodularity also plays a
role in inducing fast algorithms for graphical model inference (see Section 3.5).

There continues to be much active work on submodularity in the discrete optimization literature. There has been a surge of interest in optimizing submodular functions under various constraints, such as matroid constraints [Cal+07; LSV09; Lee+10], covering constraints [IN09], cut constraints [JB16], and other combinatorial constraints [JB11; IJB13] such as paths, st-cuts, spanning trees, and perfect graph matchings.

Most of the algorithms that optimize submodular functions are inherently sequential, meaning the algorithm steps through a sequence of decisions in series based on the outcomes of past decisions it has made. Submodular functions are inherently global and, unlike graphical models, do not necessarily allow any one set of elements to be selected without influencing the value of selecting other sets of elements. This can be seen even when considering the simple square-root submodular function $f(A) = \sqrt{|A|}$ seen above, where every element interacts with every other element, although trivially. More complex submodular functions still involve global interaction but much less trivially. This property is anathema to parallel computation where we wish, in a structure, to find a sub-structure that can be computed relatively independently of other sub-structures. Submodular functions, in general, offer no such independence-between-sub-structures property. Nevertheless, there have been efforts to develop parallel submodular optimization algorithms. In [Mir+13], for example, the ground set is partitioned, each block is optimized over separately, and then the resulting solutions are merged and optimized over again. More recently, researchers began studying the tradeoffs between approximation quality of an algorithm that proceeds in “rounds”, where each round one is allowed to perform polynomially many steps of computation. One in particular wishes to find the minimum number of sequential rounds (i.e., the minimum time) to achieve a given approximation quality where a polynomial number of computational steps (e.g., set function queries) may be performed embarrassingly in parallel, meaning each function query may be derived using results only from previous rounds but not from any results of the concurrent round thus allowing each query to occur simultaneously in parallel. The minimum number of rounds, each having polynomial cost, to achieve a given (often constant) approximation ratio is called the adaptive complexity of the problem. One wishes for algorithms that have the best (lowest) adaptive complexity for a given approximation ratio [LLV20; BS18; BBS20].

It is an exciting time for combinatorial optimization involving submodular and supermodular objectives, as many combinatorial problems that in the past have used only modular cost functions can be extended to submodular functions while still retaining polynomial time approximability; this gives combinatorial problems significantly more power and expressivity. These algorithms, especially when they are shown to be polynomial time approximable in one form or another, open the doors up to an enormous number of useful applications. A few of these applications, in the case of machine learning, are listed next.

3 Applications of Submodularity in Machine Learning and AI

Submodularity arises naturally in applications in machine learning and artificial intelligence, but its utility has still not yet been as widely recognized and exploited as other techniques. For example, while information theoretic concepts like entropy and mutual information are extremely widely used in machine learning (e.g., the cross-entropy loss for classification is ubiquitous), the submodularity property of entropy is not nearly as widely explored.

Still, in the last several decades, submodularity has been increasingly studied and utilized in the context of machine learning. It has now become an essential ingredient in many machine learning and data scientists’ book of recipes. Submodular maximization has been successfully used for selecting summaries (or sketches) of text documents [LB10a; LB11; LB12] recorded speech [LB09; Liu+13; Wei+13; Wei+14a] image compendia [Tsc+14] sets of protein sequences [LBN18], sets of genomics assays [Wei+16] and sets of genomic loci [Gas+19]. It has been used for variable/feature selection [KG05], modeling and selecting influential nodes in a social network [KKT03; KKT15], Gaussian processes [GKS05a], and active learning [GB10a; GB11a; GK10]. Submodular minimization has found use in graphical model inference [KZ04] and PAC learning [NB04], clustering [NJB05a; NB07], and sensor placement for graphical models [KG05].

Central to these papers is that some form of entropy, mutual information, and social network influence of a set of nodes in a social network are all submodular. One would also expect (intuitively) that the information capacity of subsets of features or queries could be formulated as a submodular function. Indeed, submodularity has also become a key component in active learning [Hoi+06; Kra+08; GB09; Set10; GB10b;
It is natural, therefore, to expect that results from the theory of submodular functions can be used to resolve, both, some of the theoretical and some of the practical problems arising in machine learning.

In the below we begin to provide only a brief survey of some of the major sub-areas within machine learning that have been touched by submodularity. The list is not meant to be exhaustive, or even extensive. It is hoped that the below should, at least, offer a reasonable introduction into how submodularity has been and can continue to be useful in machine learning and artificial intelligence.

### 3.1 A Summary of the History of Summarization: Sketching, CoreSets, Distillation, and Data Subset & Feature Selection

The idea of a summary goes back at least to ancient Rome, where the Latin word “Summārium” means the highest, or top most, number --- this is because numbers were added from bottom to top with the mathematical “sum” on the top row. The summary is enough of an important concept for humanity that it has been granted many different terms --- just in English, this includes abridgment, abstract, bottom line, cliff note, compendium, conspectus, digest, synopsis, outline, overview, recapitulation, rundown, and so on. In this era of big data that the fields of machine learning and artificial intelligence are currently in, a correspondingly large number of notions of summary have been developed as well. In this section, we briefly offer them a survey and taxonomy, and explain how submodularity plays a role in producing a variety of useful summarization algorithms.

A summary is a concise representation of a body of data that can be used as an effective and efficient substitute for that data. There are many types of summaries, some being extremely simple. For example, the mean or median of a list of numbers summarizes some property (the central tendency) of that list. A random subset is also a form of summary. Most of the time, however, summaries are more complex and have a specific purpose. For example, the result of a web search is a summary of the web that is relevant to the given query. All clustering algorithms are summarization procedures in that the resulting set of cluster centers (however they may be defined) summarize the data. Any machine learning procedure, in fact, can be viewed as a summarization. Machine learning is the art of telling a computer what one wants the computer to tell a second computer about a lot of data, and this takes the form of model parameters, summarizing the training data. For example, when we train an SVM, the samples corresponding to the support vectors constitute a weighted sum over a subset of samples. When we train a neural network, the parameters of the resulting model summarize the aspects of the data that are useful for mapping from input to output.

Any given summary, however, is not guaranteed to do a good job serving all purposes. Moreover, a summary usually involves at least some degree of approximation and fidelity loss relative to the original, and different summaries are faithful to the original in different ways and for different tasks. For these and other reasons, the field of summarization is rich and diverse, and summarization procedures are often very specialized.

Purposefully designed algorithms that summarize data began outside the field of machine learning. For example, in statistics, the notion of a sufficient statistic is a computation on a sample of data that, once known, renders the sample irrelevant to estimating the parameters of a distribution from which the sample was drawn. In other words, the data and model parameters are rendered independent given a sufficient statistic and, in this sense, the sufficient statistic summarizes everything about the data necessary to estimate the parameters. In statistics and computer science, random subsets are used frequently for analysis and even such agnostic computations comprise statistically unbiased summaries of the body of data being sampled. This is also true, for example, in the field of public opinion polling where the sample of people selected to answer poll questions constitutes a (hopefully) representative summary of the entire population.

Several distinct names for summarization have been used over the past few decades, including “sketches”, “coresets”, (in the field of natural language processing) “summaries”, and “distillation.”

Sketches arose in the field of computer science and was based on the acknowledgment that data is often too large to fit in memory and too large for an algorithm to run on a given machine, something enabled by a much smaller but still representative, and provably approximate, representation of the data. Viewable as a summary data structure that efficiently represents the data in some way, a sketch is computed under a given computational model. For example, in the streaming case, the data is never held in memory at the same time and instead is sequentially processed where a machine can simultaneously hold
only one (or a small number) of samples simultaneously in memory as well as the sketch being incrementally updated. This allows the data to be unboundedly, or at least unknowingly, large, but the challenge is that there is one and only one chance to view a given data sample since the algorithm is unable to go back and revisit a sample later. This includes one of the earliest sketching algorithms [FM85] that computes the number of different types of elements in a large dataset --- the data, however, is available only serially (e.g., imagine a sequence of balls arriving in some order and the goal is to count the number of distinct ball colors). Other models include the ability to merge two sketches such that the result of the merged sketch is the same as if the sketch was produced from the merged data. Linear sketches are particularly useful here since they have the property that the sketch of the sum or concatenation of two datasets is the same as the sum of the sketches. There are many sketching algorithms and sketch data structures, and usually each is developed to solve a very specific problem. For example, sketching can be as simple as counting a number of items. Normally one needs $O(\log n)$ bits to count $n$ items but when $n$ is very big, even $O(\log \log n)$ bits is too costly, especially when there are many different item types each needing to be counted. A sketching algorithm can be developed that counts using only $O(\log \log n)$ bits. Other examples of sketching include Bloom filters (a data structure that approximates set membership queries in that detecting non-membership is exact but detecting membership is only likely but not assured), detecting “Heavy hitters” (i.e., elements in a large array that are above a certain threshold), dimensionality reduction (often via the Johnson-Lindenstrauss family of results which guarantee that random projections of vectors approximately and with high probability preserve distance in a lower dimensional space as long as the lower dimensional space is not too low), and various graph based sketches. Even uniformly-at-random sampling procedures have sketching-like algorithms. Rather than load all items in just to randomly sample, one can stream them in and occasionally choose a random update in an online fashion as done by the famous reservoir sampling algorithm [Knu14]. Sketching is also useful for a variety of problems in numerical linear algebra [Lib13; Woo+14] including sketches for multiplying together very large matrices. It is almost always the case that sketching algorithms offer guarantees, often in the form of having a high $1 - \delta$ probability of having an error no more than $\epsilon$, and the computational complexity of the algorithms grows inversely with $\epsilon$ and $\delta$ (ideally poly-logarithmically). A very good sketch of sketching algorithms is given in [CY20].

Coresets are similar to sketches and there are some properties that are more often associated with coresets than with sketches, but sometimes the distinction is a bit vague. The notion of a coreset [BHIP02; AHP+05; BC08] comes from the field of computational geometry where one is interested in solving certain geometric problems based on a set of points in $\mathbb{R}^d$. For any geometric problem and a set of points, a coreset problem typically involves finding the smallest weighted subset of points so that when an algorithm is run on the weighted subset, it produces approximately the same answer as when it is run on the original large dataset. For example, given a set of points, one might wish to find the diameter of set, or the radius of the smallest enclosing sphere, or finding the narrowest annulus (ring) containing the points, or a subset of points whose $k$-center clustering is approximately the same as the $k$-center clustering of the whole [BHIP02].

Common to the coreset paradigm is that each point in the summary is assigned a weight that indicates the importance in each point. Also, in common with sketching algorithms, most coreset algorithms offer approximation guarantees where the size of the coreset depends inversely on an error $\epsilon$ and possibly (but ideally not) on the dimensionality of the points. Soon after their introduction, coresets became useful in machine learning, e.g., the core-SVMs of [Tsa+05] that facilitate the use of SVMs on larger datasets by identifying a coreset. More recently, the notion of coresets and summarization have been used for many specific applications in machine learning, good surveys and examples are in [JMF19; Fel20; WIB15; MS18], the last of which categorizes four types of coreset constructions for machine learning: geometric, gradient descent, random sampling, and sketching. In the sketching case, the coreset is viewed as a form of dimensionality reduction in data space which is like a transpose of dimensionality reduction in feature space (more on this when we discuss distillation below).

Document summarization became one of the most important problems in natural language processing (NLP) in the 1990s although the idea of computing a summary of a text goes back much further to the 1950s [Luh58; Edm69], also and coincidentally around the same time that the CliffsNotes [Wik21] organization began. There are two main forms of document summarization [YWX17]. With extractive summarization [NM12], a set of sentences (or phrases) are extracted from the documents needing to be summarized, and the resulting subset of sentences, perhaps appropriately ordered, comprises the summary. Extractive summarization therefore is a subset selection problem, where if $V$ represents the set of all sentences,
we wish to find a subset $X \subseteq V$ that represents $V$ and in particular $X$ must represent everything not selected $V \setminus X$. In an extractive summary, each sample is a genuine sentence from the original and so there is no need to ensure that the summary sentences are grammatical or factually accurate.

With abstractive summarization [LN19], on the other hand, the goal is to produce an “abstract” of the documents, where one is not constrained to have any of the sentences in the abstract correspond to any of the sentences in the original documents. With abstractive summarization, therefore, the goal is to synthesize a small set of new pseudo sentences that represent the original documents. CliffsNotes, for example, are abstractive summaries of the literature being represented. Conceptually, abstractive summarization is more natural and flexible, but it is a computationally more challenging task since one must ensure that the synthesized sentences are grammatical, natural, relevant, and factual. Indeed, there is research that compares extractive with abstractive summarization and that report “factual hallucinations” in the abstractive summaries [May+20; Kry+20], and that finds that extractive summarization is often better than abstractive due to its inherent faithfulness and factual-consistency [Hua+20; DHD20]. Extractive summarization is considerably easier computationally since the process involves only picking and choosing sentences. With abstractive summarization, one must synthesize and regenerate new sentences, similar to language translation. With extractive summarization, however, it can be more difficult to piece together the extracted sentences into a coherent paragraph or whole article, since the selected sentences might just not flow well together as a text. With abstractive summarization, the sentences can be composed for the purposes of being a coherent and fluid whole, with clarity, organization, voice, grammar, and even style. It is also possible for an abstractive summarization to be more concise since in any accurate extractive summarization there might be redundancies that are impossible to remove without either changing the sentences or removing relevant information. Therefore, there are tradeoffs between abstractive and extractive summarization. In fact, extractive summarization is often used as the first step of abstractive summarization in NLP including [Pil+20; GDR18; Liu+18; Hsu+18; Li+21] --- interestingly, there is evidence that this might even be a mechanism used by human summarizers [JM99] where extractions are done first before concept merging and resynthesis into an abstractive summary later.

Another useful variant of summarization commonly encountered in the text domain is called update summarization [DO09]. Here, the assumption is that a person has already read a set of articles and is interested only in a summary of any updates, or any new information, that has happened that is not in the articles that have already been read. Update summarization is natural in document summarization since at any given time there are too many articles to read, but a human does not start from zero knowledge, rather the human starts from having read articles up to a previous time point. Update summarization can be either extractive or abstractive.

A big part of document summarization research is in developing automatic ways to judge the quality of a summary, the reason being that obtaining human judgments of summaries is even more challenging than the human labeling tasks. This is because the human now needs to judge not just what objects or concepts lie within each sample, but instead needs to examine a large sample collection and tell if it is representative of the whole. Due to this difficulty, accurate automated summary assessment algorithms are extremely valuable. One strategy used for document summarization requires a set of ground truth reference summaries of a collection of documents, and all new candidate summaries are judged against statistics within these references. Since there can be many different summaries all of which are equally good, one strategy to do this is via n-gram statistics. A classic example of this approach is the ROUGE metric [Lin04]. The ROUGE-N recall metric can be written as the following set function:

$$f_{\text{ROUGE-N-Recall}}(S) \equiv \frac{\sum_{i=1}^{K} \sum_{e \in R_i} \min(c_e(S), r_{e,i})}{\sum_{i=1}^{K} \sum_{e \in R_i} r_{e,i}},$$

where $K$ is the number of reference summaries, $R_i$ is the set of sentences in the $i$th reference summary, $e$ is a particular n-gram, $c_e(S)$ is the number of times n-gram $e$ occurs in a hypothesized set of sentences $S$, and $r_{e,i}$ is the number of times n-gram $e$ occurs in reference summary $i$. Since $c_e(S)$ is non-negative monotone and $\min(x, a)$ is a concave non-decreasing function of $x$, $\min(c_e(S), r_{e,i})$ is monotone submodular since it is a monotone non-decreasing concave function composed with a modular function. Since summation preserves submodularity, and the denominator is constant, we see that $f_{\text{ROUGE-N-recall}}$ is monotone submodular, as was shown in [LB11]. That ROUGE-N is submodular does not mean that it can be used to produce a summary,
since it is instantiated from human summaries. Rather it is used only to judge a hypothesized summarization that has not had the opportunity to benefit from the human reference summaries (if it did, it would be like training on the test set). On the other hand, that such a widely used metric is submodular provides evidence of the naturalness of submodularity for judging summary quality, further discussed below.

Another form of summarization that has more recently become popular in the machine learning community is data distillation [SG06; Wan+20; Suc+20; BYH20; NCL20; SS21; Ngu+21] or equivalently dataset condensation [ZMB21; ZB21]. With data distillation⁴, the goal is to produce a small set of synthetic pseudo-samples that can be used, for example, to train a model. The key here is that in the reduced dataset, the samples are not compelled to be the same as, or a subset of, the original dataset. This is akin to the difference between the k-means algorithm (which is a form of data distillation) and the k-medoids algorithm (which is a form of extractive summarization or unweighted coreset). Data distillation therefore is the same as abstractive summarization but on arbitrary data modalities (e.g., images). Some references even consider sketchings to be data projections [MS18; TBA19] and thus data distillation --- for example, if we pre-multiply an \( n \times m \) design matrix \( X \) by a \( k \times n \) projection matrix \( P \), we get a resulting “sketched” \( k \times m \) matrix \( PX \) that can be thought of as having \( k \) linear distilled samples in the same dimension-\( m \) feature space as the original design matrix, and hence we can view this as dimensionality reduction in data space. The above cited methods correspond to non-linear distillation procedures produced by taking gradients, with respect to the data samples being learnt, of an objective that involves a deep neural network, and usually involve implicit gradients [Wan+20; ZMB21]. Sometimes the objective is based on kernel ridge regression using a kernel obtained from a neural network via the neural tangent kernel [NCL20]. With any form of data distillation, a large dataset is distilled down to a smaller synthetic or pseudo-sample dataset.

All of the above should be contrasted with data compression, which in some sense is the most extreme data reduction method. With compression, either lossless or lossy, one is no longer under any obligation that the reduced form of the data must be usable, or even recognizable, by any algorithm or entity other than the decoder, or uncompressed, algorithm. The compressed data is thus unrecognizable, looks like uniformly-at-random bits, and is unusable unless decompressed back to its original form. So, while the compressed form of the data might be very small, the data is not useful in this form until one expands it back to its original large size. This is different from summarization procedures which require that the data is useful immediately in its summarized form without re-expansion. Unlike compression, summarization procedures also have no requirement that the original data, either exactly or approximately, must be reconstructable back from the summary. Compression can be slow for larger datasets but might be faster than data distillation since compression is not obliged to keep the data in a form that can be used like the original. Compression therefore is meant for other tasks, specifically storage and communication.

What then precisely is the difference between summarization, sketching, coresets, and distillation? It is challenging to come up with a clear distinction between the methods. This gets even more convoluted because, for example, there are core set algorithms for the \( k \)-means procedure [BLK18] (i.e., how to reduce a dataset so that running \( k \)-means on the reduced dataset produces the same answer as when \( k \)-means is run on the entire dataset), but then the resulting \( k \)-means set itself can be seen as a coreset --- running \( k \)-means on the result of \( k \)-means will produce the same answer. This is also true for \( k \)-center [BHP12] and other clustering procedures.

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⁴Data distillation is distinct from the notion of knowledge distillation [HVD14; BC14; BCNM06] or model distillation, where the “knowledge” contained in a large model is distilled or reduced down into a different smaller model.
### 3.1.1 Summarization Algorithm Design Choices

It is the author’s contention that the notions of summarization, coresets, sketching, and distillation are certainly analogous and quite possibly synonymous, and they are all different from compression. The different names for summarization are simply different nomenclatures for the same language game. What matters is not what you call it but the choices one makes when designing a procedure for summarization. And indeed, there are many choices.

We next summarize (or distill) the choices available to make when considering or designing a summarization procedure and discuss their uses, advantages, and disadvantages. These choices for summarization are summarized in Figure 3.

- **Parallelizable and/or distributed construction or centralized.** This first choice has little to do with the type of summarization and instead what a given summarization algorithm offers in terms of its natural ability to be parallelized. Hence, we do not discuss this further other than to say that it is of course desirable to have algorithms that are easy to be efficiently parallelized.

- **Problem specific or a universal framework.** As mentioned above, many of the corset and sketching algorithms are developed for a specific geometric or algorithmic problem in mind and have guarantees associated only with that specific problem. The algorithmic approaches can be very different from each other, and they also have very different approximations. We might, however, conceive of a framework that is more universal, where the same algorithmic framework can be used to produce a coreset for a variety of different problems and where the algorithmic framework is parameterized in some way. Indeed, this is the strategy for submodular summarization as discussed further below, where the submodular function itself acts as a parameter to the summarization procedure which is done using the same algorithm.

- **Query specific or generic.** Sometimes it is desirable for a summary to be generic, in an attempt to capture as much about a dataset as possible and be ready to answer any query that might be asked of the original. This can be useful when one does not know the purpose of a summary beforehand. On the other hand, a smaller, more direct, specific, and focused summary can be produced if a query is available at summarization time. The classic example, as mentioned above, is web search, where we extractively summarize the web in response to a web search query; generic web summarization would not be very useful (e.g., a diverse top ten web page list is unlikely to solve many problems) but query-specific web summarization is the basis for billion-dollar businesses.

- **Streaming, Batch, or Mini-batch samples or indirect (no samples) input.** If it is possible to load all of the data into memory simultaneously and be given random access to all samples, this affords an algorithm the greatest opportunity to produce a better summary. However, as mentioned above in the context of sketching, this is often infeasible for large datasets or when all the data is not available at a given time. A solution to this problem is to stream data sequentially. Often, however, the data need not be streamed one sample at a time, but rather one batch at a time, so an algorithm holds, at any point in time, both the summary and one (or perhaps two) batches of data. While a batch is in memory, random access over that batch is granted, but once a batch is removed from memory is never again accessible, although samples within the batch might have been placed in the summary.

A summary can also be produced not directly from the data, but instead via an intermediate representation that was computed from the data beforehand. That is, an indirect summarization means that the summary is produced by some structure other than the original samples. For example, the summary might be produced from a model that has been trained on the data, but when the data is no longer available. One example of this achieves knowledge distillation via indirect data distillation using a pre-trained fixed glass-box teacher model [Yin+20], hence, this is a way of achieving knowledge distillation by first recovering samples directly from a model that had previously been trained on data, but the data is not available (most data distillation methods require the training data to still be available). This process is related to the privacy worry that exists about neural networks, i.e., that it is sometimes possible reconstruct the training data (or something that mimics and “summarizes” the training data) using access only to the model, or some property of the model such as its gradients (see [ZLH19] and [Hua+21] in a federated learning context). Another imaginary example would be to...
ask GPT-3 or any other modern foundation models to "Please summarize the book War and Peace" and it will produce some form of summary where the quality will depend on the extent the model has memorized the information from that book.

- Weighted or unweighted samples. As mentioned above, a core feature of coresets is that the resulting summary consists of weighted samples indicating how important each sample is, but a summary might also take the form of unweighted samples. In the indirect summarization strategy, there are no samples, so this distinction does not apply.

- Extractive subset or synthesized distilled abstractive. This is one of the most interesting of choices for a summarization procedure and corresponds to the difference between abstractive vs. extractive document summarization and also the difference between data distillation vs. subset selection that we saw above.

Extractive summarization and coresets have a number of important properties. For example, one is guaranteed that the data samples have the same form and style as the original data, and that all samples are natural, since the summary is a subset of the original. Hence, there can be no aberrational samples, in the same sense that a median is an original sample unlike a mean. Since one is constrained to be a subset of the original, a summary of a given size has less opportunity to retain the information in the original as a distillation strategy. The reason is that it is possible that any pair of samples are partially redundant with respect to each other (this can be made precise using submodular functions where for any \( v, v' \) we have \( \max(f(v), f(v')) < f(v, v') < f(v) + f(v') \)). On the other hand, extractive summarization has the greatest opportunity to be fast, since subset selection is computationally relatively easy (compared to abstraction) since the summary is always a subset of the original. We say relatively since, in the most general case, there are still an exponential, in \( k \), number of size-\( k \) subsets of a set of size \( n \). This is again something submodularity helps with as seen below.

In contrast, abstractive summarization (or data distillation, or sketching) have different properties than the above. Here, it is still guaranteed that the data has the same form as the original and, unlike compression, the summary can be used and viewed as if it was a subset of the original. There is some chance, however, that the synthesized samples are unlike any of the original, in the same sense that a mean might be unlike any of the original points and could live in a region of very low probability when the distribution is multimodal. Hence, a synthetic sample has the chance of being unnatural and uninterpretable (this is discussed further below). Abstractive summarization offers the greatest chance to reduce the size of the summary while preserving information (since it is not constrained to have the summary be a subset). Thus, abstractive summarization is like a hybrid between extractive summarization (where the samples of the summary are all real) and compression (where the compressed form is not constrained to use a representation resembling samples at all). Like compression, abstract summarization is also computationally challenging. Even compression, however, can be computationally easier than abstractive summarization since compression is not constrained to have the compressed representation resemble samples in the original form. Therefore, abstract summarization (data distillation) is the most difficult, since we want (and have the opportunity) to make the smallest set possible while ensuring the summary is immediately useful in its summarized form.

Lastly, we mention that subset selection and synthesized summaries are not required to be exclusive. It is conceivable to get the best of both worlds by producing a summary that consists of some samples from the original augmented by some additional samples that are synthesized. Indeed, in human-produced document summarizations, sometimes there is nothing better than to quote the original, other times it is best to paraphrase, and in many cases, it is best to do both.

- **Interpretable samples vs. anything goes.** Interpretability has become an important research topic in machine learning, where it is desirable to be able to interpret and understand the decisions made by a large complex AI system. Another design choice for a summarization procedure is whether or not the summary should be interpretable, and this can take the form of the individual samples being interpretable and natural or the entire sample being collectively coherent. We first discuss the former and then the latter.
As mentioned above, extractive summarization ensures that the summary consists of natural samples since the samples are all from the original. Abstractive summarization, however, might produce a summary where the synthetic pseudo-samples are unnatural, hallucinatory, or factually inconsistent. Regardless, the choice between interpretable vs. “free” is application dependent. For example, in the NLP domain, emphasis is placed on the synthesized samples being factual and natural since the typical end user of the summary is a human reader. Effort must therefore be placed on ensuring that the distilled samples have this property, leading to the aforementioned increase in computation.

For other applications, however, interpretability might or might not be less important. The data distillation examples shown in [Wan+20] look distorted and unnatural even though they train a model well. If a corresponding degree of distortion existed in an abstractive document summarization example, the results would be unacceptable to a human reader. In computer vision, hallucinatory concepts in distilled data might mean a bundle of pixels are set to values that one would never find in a real image, but if it helps the training of a classifier, the distortion might not matter. In abstractive document summarization, if a random grammatically correct but factually nonsensical phrase “Dogs swim on the roof of Seattle” appears, it would not be useful for a human-indented summary, but perhaps such hallucinatory phrases could be useful to train a text classification system or for a large language model. There have not, as of yet, been many studies on abstractive data distillation for the purposes of training a text classifier model save for [SS21] and a few others. The results of [ZMB21; NCL20] show fairly realistic looking synthetic samples, but even here we see some distortion that might not be acceptable in a human-consumed document summarization. Therefore, the choice between interpretable vs. “free” depends on the reason for doing summarization.

Now, one might think that factual inconsistency and naturalness do not matter when producing a distilled dataset for the purpose of training another model. The distilled samples might not need to resemble any of the original samples since, when the goal is classification, it matters only that the dataset retains the key distinctive properties of each class relative to other classes. This is the same idea as “structural discriminability” as shown in Figures 5 and 6 of [Bil+01] which is analogous to Figure 3 in [Wan+20], and Table T12 in [ZMB21]. In [ZMB21], for example, a generated synthetic summary is compared between a GAN and their method and while it was found that their method did a better job in terms of training a new model, it was speculated that the reason was that the GAN’s purpose was to generate realistic-looking images, but not to train an accurate model.

One might reasonably say that, for classification purposes, only the structurally discriminative aspects of a dataset need to be captured in a distilled dataset if one wants the smallest possible summary. In other words, the smallest summary retains only minimum information necessary, and here that information means the distilled data retains only that which distinguishes different classes from each other. Anything irrelevant to achieving high classification accuracy is stripped away.

On the other hand, as with document summarization, we still may wish to retain the factual consistency and naturalness that one automatically gets with extractive summarization. There are several reasons for this. Firstly, we may wish for the summary itself to be interpretable by humans, for the same reason we would wish any AI model to be interpretable. Having an interpretable summary can even improve interpretability of any subsequently trained model on that data. This may be particularly important when debugging the ML training process --- it becomes harder to debug depending on the degree to which the images in the synthesized dataset do not look natural. One of the properties of computer vision that makes it an attractive domain within which to perform machine learning research relative to other domains, such as biology, sensors (e.g., radar, lidar, or sonar), financial records, and so on, is that humans have cognitive capabilities that help them debug the results. It is estimated that between 20% and 30% of the cortex in humans is devoted to visual processing [SY16] and this can only help when debugging computer-vision based machine learning systems, especially with the synergy possible when the final training data looks realistic and natural.

Secondly, and more importantly, there is a danger that the distilled summary contains only the non-robust features of the training data that are sufficient to obtain good accuracy on a test set not because the summary captures important information about the objects being classified but only because it captures aspects in the data set that are associated with those objects. An extreme example of this is shown in [Ily+19; GH19] where it is implied that the hallucinatory results in synthetic
samples matter very little when wishing to train a model that performs well. This work shows that by producing a synthetic training dataset that uses only the ‘non-robust’ features of the data, they can train other models that work well even though the samples look entirely wrong to a human. For example, synthesized images that appear as dogs may be labeled as cats, and synthesized images that look like cats might be labeled as dogs. These images have been modified in adversarial ways to look, to a model, like their real label. When those images become the training data, the resulting model works reasonably well. These images take advantage of the opportunistic tendency when training large neural networks to associate the easiest signal in the input as possible with the correct label. There is much research into the lack of robustness that some models have since, during training, they associate wrong cues in the input with output labels [GH19]. While such work does not have abstractive summarization or distilled data as its goal, it is very relevant. The reason is that it shows it is possible to produce synthetic samples that look very different from natural samples but that still can be used to train a model.

This poses a danger for data distillation as well since there is no reason, moreover, that distilled data is immune to these effects unless special provisions are made. In some sense, adversarial samples that look identical to real samples but that fool a model into making a wrong decision are the dual of synthetic abstractive factually-inconsistent samples that fool a model into learning a correct decision. Of course, such factually-inconsistent images do not represent the original samples since they are adversarially produced to take advantage of a model training’s tendency to focus on the wrong part of an image when learning to associate with a label. Hence, the goal in NLP’s abstractive summarization to avoid such hallucinatory artifacts is a good one as well for any machine learning task when one wishes to summarize, where the summary is supposed to represent the original.

It was mentioned above that for NLP’s abstractive summary, the set of sentences ideally can be ordered to make a coherent text with long-range interactions. Another form of interpretability of a summary is to consider the gestalt of the entire summary itself. One can imagine that either extractive or abstractive summarization has the chance to produce a coherent summary on the whole, but abstractive summarization being less constrained than extractive summarization has more opportunity to do so.

To summarize the past two choices (i.e., Figure 3-6.x and -7.x), if one wants to guarantee that the samples are natural, extractive summarization (subset selection) is easiest. If computation is at a premium or if the data set sizes are massive, then extractive summarization is best. If one wants the absolute smallest possible summary for a given amount of information, and one is not worried about interpretability of the samples and allows for structurally discriminative samples, then data distillation is best since there is more opportunity for compression. If one wants to ensure the samples produce a summary that constitutes a coherent whole, and if computation is not the primary concern, then abstractive summarization is best.

- Constraint type (size or other structure). We almost always want a summary to be small, and this can be seen as a constraint on the cardinality of the summary. In other cases, we may wish the summary to satisfy other constraints as well. For example, the summary might comprise a tree or a sequence in some space, or the sum of the costs of each of the summary items might need to be below some budget (e.g., as in a knapsack constraint), or we might wish the summary to collectively be coherent so that summary elements can be organized into a good presentation (as in abstractive document summarization, where the summary sentences together must be able to produce a good text). In all of these cases, we can view this as an additional constraint on or quality required of the resulting summary.

A distinction not included in Figure 3 is that of supervised vs. unsupervised. This means, when each element in a set to be summarized is a data sample, if the summarization procedure uses a feature-label (x, y) pair, or if it uses just the features (x). This distinction is specific to the problem of summarizing a training set for the purposes of classification or regression, and not a more general summarization goal. Another distinction not given in the figure is that of update summarization, but if it were added it could be located at a hypothetical Fig. 3-3.3, but this is not ideal. The reason is that update summarization can be seen as a form of “anti-query” focused summarization since the summarization in this case should, if anything, neglect information relevant to what is already known, and the summary should be focused only on what
is new. It is also the case that one might want both to focus on a particular query and neglect a particular anti-query, so therefore it would be better to consider update-summarization as part of Fig. 3-3.3. How is submodularity situated within this sea of summarization strategies shown in Figure 3? In fact, submodular summarization procedures touch all options except for Fig. 3-4.4 (indirect summarization), Fig. 3-6.2 (abstractive summarization), and Fig. 3-7.2 (obscure samples). The reason is that a submodular function is a set function, and producing a summary (or coreset, or sketch) of a ground set $V$ corresponds to producing a subset of that ground set. Hence, there is no immediate way for a submodular function to bypass the data (4.4), produce an abstractive summary (6.2), or to suffer from obscure and/or hallucinatory samples (7.2) (although there is a chance to select outliers).

It is however odd that in much of the sketching and coreset literature, the connections to a submodular summary does not more frequently arise. In some cases, when it comes up, it is not for the purposes of using submodularity to create a sketch, but rather to sketch a particular submodular function itself [Goe+09; BH11; Bal+12; Bad+12; CD17; YZ19]. This is essentially the problem of how to approximate a given submodular function using a relatively small number of oracle function queries.

On the other hand, submodularity offers essentially an infinite number of ways to perform data sketching and coresets. When we view the submodular function as an information function (as we discussed in Section 3.2), where $f(X)$ is the information contained in set $X$ and $f(V)$ is the maximum available information, finding the small $X$ that maximizes $f(X)$ (i.e., $X^* \in \arg\max\{f(X) : |X| \leq k\}$), is a form of coreset computation that is parameterized by the function $f$ which has $2^n$ parameters since $f$ lives in a $2^n$-dimensional cone. Performing this maximization will then minimize the residual information $f(V \setminus X|X)$ about anything not present the summary $V \setminus X$ since $f(V) = f(V \cup V \setminus X) = f(V \setminus X|X) = f(X) + f(V)$ so maximizing $f(X)$ will minimize $f(V \setminus X|X)$. For every $f$, moreover, the same algorithm (e.g., the greedy algorithm) can be used to produce the summarization, and in every case, there is an approximation guarantee relative to the current $f$, as mentioned in earlier sections, as long as $f$ stays submodular. Hence, submodularity provides a universal framework for summarization, coresets, and sketches (Fig. 3-2.2) to the extent that the space of submodular functions itself is sufficiently diverse and spans over different coreset problems. This is promising since even within one class of submodular function, e.g., with just the facility location function, there is enormous flexibility and expressivity in terms of what similarity measure to use and how to parameterize that similarity measure. But the facility location, as mentioned in Section 2.2 is only one of many submodular functions.

Ordinarily, one would expect a summary to necessarily lose fidelity relative to an original larger dataset. On the other hand, with a submodular perspective it is possible for the summary to lose no information relative to the original. For example, assuming the submodular objective is the correct summary objective, then given two sets $A \subset B$ with $f(A) = f(B)$, there is no reason to prefer $B$ over $A$ since $B$ is partially redundant. That is, $f(B|A) = f(A + B) - f(A) = f(B) - f(A) = 0$, the additional samples in $B$ not in $A$ are redundant relative to those already in $A$. Also, a summary can be preferable to the whole due to bias removal. If the whole $V$ is biased or imbalanced (i.e., if there are over-represented majorities and under-represented minorities within the whole), a summary can re-balance the data so that concepts have a more equal and balanced representation. For example, one might find the value per item $f(V)/|V|$ of the whole to be smaller than the value per item in the summary $f(A)/|A|$. This suggests algorithms to optimize the ratio of submodular functions, as has been addressed in [Bai+16]. For these reasons, we sometimes see machine learning performance increase when trained on a subset than when trained on the whole albeit it is usually the case that the subset in such cases is about 80% to 90% of, i.e., not that much smaller than, the whole.

Overall, the corset or sketching problem, when using submodular functions, therefore becomes a problem of “submodular design.” That is, how do we construct a submodular function that, for a particular problem, acts as a good coreset producer when the function is maximized. There are three general approaches to produce an $f$ that works well as a summarization objective: (1) a pragmatic approach where the function is constructed by hand and heuristics, (2) a learning approach where all or part of the submodular function is inferred from an optimization procedure, and (3) a mathematical approach where a given submodular function when optimized offers of a coreset property.

3.1.2 Crafting a Submodular Function By Hand

When the primary goal is a practical and scalable algorithm that can produce an extractive summary that works well on a variety of different data types, and if one is comfortable with heuristics that work well
in practice, a good option is to specify a submodular function by hand. For example, given a similarity matrix, it is easy to instantiate a facility location function and maximize it to produce a summary. If there are multiple similarity matrices, one can construct multiple facility location functions and maximize their convex combination. One can utilize feature-based functions to ensure that the summary is diverse with respect to a set of qualities represented by the features or combine such a feature-based function with the above mixture of facility location functions to produce a richer summarization objective. It is also easy to mix in a modular function when one wishes to ensure that the summary is relevant to a particular query or that has a particular quality. That is, one might take a combination of a diversity component (which is a mixture of submodular functions to appropriately capture diversity) along with a relevance modular component (to ensure the summary is relevant to a query). As an example, we might be interested in image summarization, but preference should be placed on those images with human faces. A modular function \( m \) can be used to express the probability that an image contains a face, and \( m(X) \) corresponds to the overall face quality in set \( X \). Maximizing this alone, however, would lead to a redundancy since \( m \) is only a modular function --- e.g., consider an image with a high face score that is duplicated and thus selected multiple times. But maximizing \( \lambda m(X) + (1 - \lambda)f(X) \), where \( f(X) \) is a mixture of facility location functions and thus indicates the diversity in set \( X \) will produce a summary consisting of a diverse set of faces, assuming \( \lambda \) is set appropriately.

Such a strategy for producing a summary might involve a number of hyperparameters that need to be tuned, \( \lambda \) being only one of them. Hyperparameter tuning would need to occur in the same way that hyperparameter are always tuned, i.e., via a search strategy that evaluates performance on a validation set, and there are many search strategies available (e.g., genetic algorithms, Bayesian methods, grid search with early pruning, and so on). It should be clear that even after tuning, and while the resulting function is submodular, performing submodular maximization on the summarization objective offers a mathematical guarantee regarding the quality of the resulting set relative to the objective, and not necessarily relative to the original problem (i.e., the true quality of a summary as judged, say, by a human or a machine learning model). Hence, the hyperparameter tuning must be done appropriately.

Still, this is viable and practical and has been used successfully many times in the past for producing good summaries. One of the earliest examples of this is the algorithm presented in [KKT03] that shows how a submodular model can be used to select the most influential nodes in a social network. Perhaps the earliest example of this approach used for data subset selection for machine learning is [LB09] which utilizes a submodular facility location function based on Fisher kernels (gradients w.r.t. parameters of log probabilities) and applies it to unsupervised speech selection to reduce transcription costs. Other examples of this approach includes: [LB10a; LB11] which developed submodular functions for query-focused document summarization; [KB14] which computes a subset of training data in the context of transductive learning in a statistical machine translation system; [LB10b; Wei+13; Wei+14b] which develops submodular functions for speech data subset selection (the former, incidentally, is the first use of a deep submodular function and the latter does this in an unsupervised label-free fashion); [SS18a] which is a form of robust submodularity for producing coresets for training CNNs; [Kau+19] which uses a facility location to facilitate diversity selection in active learning; [Bai+15; CTN17] which develops a mixture of submodular functions for document summarization where the mixture coefficients are also included in the hyperparameter set; [Xu+15] uses a symmetrized submodular function for the purposes of video summarization (see below).

We note that some of the above methods are generic (Fig. 3.3.2) while others are query focused (Fig. 3.3.1) and some are supervised while others are unsupervised.

One last thought on the by-hand submodular crafting approach. Like any empirical endeavor, such as most deep learning research, when developing a submodular function for the purpose of summarization, it is important to establish careful, competitive, and state-of-the-art baselines to ensure that the submodular function being utilized is working as well as possible. Metrics to compare include both the summarization quality but also the underlying computational effort needed to perform the summarization.

### 3.1.3 Learning a Submodular Function

The learnability and identifiability of submodular functions has received a good amount of study from a theoretical perspective. The fundamental question in this setting is how the quality of the resulting learnt function is judged. Moving from most challenging to most accommodating, this includes how should the function being learnt approximate the true submodular function, should the learning take place in certain
subfamilies of submodular functions, and if all aspects of a target submodular function itself should be learnt or if it is acceptable to learn only some aspects (e.g., sets with large value).

Starting with the strictest learning settings, the problem looks pretty dire. For example, [SF08; Goe+09] shows that if one is restricted to making a polynomial number of queries (i.e., training pairs of the form \((S, f(S))\)) of a monotone submodular function, then it is not possible to approximate \(f\) with a multiplicative approximation factor better than \(\tilde{O}(\sqrt{n})\). In [BH11], goodness is judged multiplicatively, meaning for a set \(A \subseteq V\) we wish that \(\tilde{f}(A) \leq f(A) \leq g(n)f(A)\) for some function \(g(n)\), and this is typically a probabilistic condition (i.e., measured by distribution, or \(\tilde{f}(A) \leq f(A) \leq g(n)f(A)\), 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 \(\text{err}_p(f, \tilde{f}) = \|f - \tilde{f}\|_p = (E_{A \sim P_i}[|f(A) - \tilde{f}(A)|^p])^{1/p}\), we may wish \(\text{err}_p(f, \tilde{f}) < \epsilon\) 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 [BH11], we also “mostly” \(\beta > 0\) learn. In some cases, we wish to learn the best submodular approximation to a non-submodular function. In other cases, we are allowed to deviate from submodularity as long as the error is small. Learning special cases includes coverage functions [FK14; FK13], and low-degree polynomials [FV15], curvature limited functions [JB13], functions with a limited “goal” [DHK14; Bac+18], functions that are Fourier sparse [Wen+20], or that are of a family called “juntas” [FV16], or that come from families other than submodular [DFF21], and still others [BRS17; FK14; FK17; FK20; FK13; YZ19]. Other results include that one cannot minimize a submodular function by learning it first from samples [BS17]. The essential strategy of learning is to attempt to construct a submodular function approximation \(\hat{f}\) from an underlying submodular function \(f\) querying the latter only a small number of times. The overall gist of these results is that it is hard to learn everywhere and accurately.

In the machine learning community, learning can be performed extremely efficiently in practice, although there are not the types of guarantees as one finds above. For example, given a mixture of submodular components of the form \(f(A) = \sum_i \alpha_i f_i(A)\), if each \(f_i\) is considered fixed, then the learning occurs only over the mixture coefficients \(\alpha_i\). This can be solved as a linear regression problem where the optimal coefficients can be computed in a linear regression setting. Alternatively, such functions can be learnt in a max-margin setting where the goal is primarily to adjust \(\alpha_i\) to ensure that \(f(A)\) is large on certain subsets [SSJ12; LB12; Tsc+14]. Even here there are practical challenges, however, since it is in general hard in practice to obtain a training set of pairs \(\{(S_i, F(S_i))\}\). Alternatively, one also “learn” a submodular function in a reinforcement learning setting [CKK17] by optimizing the implicit function directly from gain vectors queried from an environment. In general, such practical learning algorithms have been used for image summarization [Tsc+14], document summarization [LB12], and video summarization [GGG15; Vas+17; Gon+14; SGS16; SLG17]. While none of these learning approaches claim to approximate some true underlying submodular function, in practice, they do perform better than the by-hand crafting of a submodular function mentioned above.

### 3.1.4 Submodularity Based CoreSets

By a submodularity based coreset, we mean one where the direct optimization of a submodular function offers a theoretical guarantee for some specific problem. This is distinct from those cases in Sections 3.1.2 and 3.1.3 where the submodular function is used as a surrogate heuristic objective function and for which, even if the submodular function is learnt, optimizing it is only a heuristic for the original problem. Here, the goal is to find a submodular function so that, under its maximization using, say, the greedy algorithm, we can show an approximation for some underlying problem.

In some limited cases, it can be shown that the function we wish to approximate is already submodular, e.g., in the case of certain naïve Bayes and k-NN classifiers [WIB15] where the training accuracy, as a function of the training data subset, can be shown to be submodular. Hence, maximizing this function offers the same guarantee on the training accuracy as it does on the submodular function. Unfortunately, the accuracy function for many models is not submodular, although they do have a difference of submodular [NB05; IB12] decomposition.

In other cases, it can be shown that certain desirable coreset objectives are inherently submodular. For example, in [MBL20], it is shown that the normed difference between the overall gradient (from summing
over all samples in the training data) and an approximate gradient (from summing over only samples in a summary) can be upper bounded with a supermodular function that, when converted to a submodular facility location function and maximized, will select a set that reduces this difference, and will lead to similar convergence rates to an approximate optimum solution in the convex case. A similar example of this in a DPP context is shown in [TBA19]. In other cases, subsets of the training data and training occur simultaneously using a continuous-discrete optimization framework, where the goal is to minimize the loss on diverse and challenging samples measured by a submodular objective [ZB18]. In still other cases, bi-level objectives related to but not guaranteed to be submodular can be formed where a set is selected from a training set with the deliberate purpose of doing well on a validation set [Kil+20; BMK20]. Overall, this area of research is quite nascent as of this writing and it is believed that there will be many more coreset-producing submodular showcases in the future.

3.1.5 Advantages to Submodularity as a CoreSet Paradigm

Regardless of how a submodular is produced as an objective to produce a coreset, there are a number of potential advantages and a few disadvantages.

First, this approach allows us to focus on the parameter of the coreset producer, namely the submodular objective $f$, rather than the algorithm stays fixed throughout the search. Regardless of the objective, therefore, one maintains essentially the same computational cost for a given coreset problem (assuming that evaluating the candidate objectives also stays the same). Moreover, once we have found the right $f$, we immediately have a guarantee associated with the guarantee provided by a submodular optimization algorithm.

Secondly, as seen above, there are many ways to partially parameterize a submodular function in fewer dimensions than the $2^n$ dimensions associated with the submodular cone. Submodularity is closed under convex mixtures, so a coreset objective can be formed as $f(A) = \sum_i \alpha_i f_i(A)$ a weighted sum of specific objectives. Alternatively, robust versions can be constructed of the form $f(A) = \min_i f_i(A)$ --- this later case is not submodular but there are fast algorithms for maximizing the minimum of a set of submodular functions available [Kra+08; Tzo+17; OSU18]. In either case, it also is easy to add modular functions to the mix to generate individual item costs as well, all while staying within the same paradigm.

Since a primary algorithm for maximizing a submodular function is greedy, then prefixes of summaries are still summaries. This contrasts with, for example, data distillation methods, when one wishes a summary of size $k$, one must optimize a summary of size $k$ --- as mentioned in [NCL20; Ngu+21], selecting a summary of size smaller than $k$ from a distilled data set of size $k$ is suboptimal. In the submodular approach, however, the greedy algorithm gives an ordering $s_1, s_2, \ldots$ so that a summary if $k$ is $S_k$ and is a prefix of the ordering. Hence if you already have a summary of size $k$ and kept track of the order while running the algorithm, a summary of size $k'$ for all $k' < k$ is immediately available.

Another advantage of the submodular approach is that there are many types of constraints besides a cardinality constraint that the resulting summary might need to satisfy and there are simple modifications to the objective that result in update summarization. Regarding other constraints, this includes matroid (where the summary must be an independent of a matroid), intersection of matroids (where the summary must be independent in multiple matroids), knapsack (where the summary must not have a cost that exceeds a given budget), and combinatorial constraints (where the summary might need to be a tree, a cycle, a cut, or some other combinatorial structure), or combinations thereof. For all of these types of constraints there are algorithms that usually have theoretical guarantees and often work quite well in practice. Regarding objective modifications, defining a function $g(A) = f(A | B)$ for a given fixed set $B$ preserves submodularity. If $g(A)$ is then maximized, the result are those items that are both diverse but not already explained by $B$, which is precisely the goal of update summarization. For example, suppose $B$ is a summary of newspaper articles that have already been read, and we utilize $g(A)$ as the objective over a set of new articles. The result will be a subset of articles that are both diverse and new relative those already read articles $B$. Such an objective modification is not unrelated to the combinatorial mutual information described further below.

Several other advantages include that it is relatively easy to produce random diverse samples from any submodular function, very much like a DPP. For example, there are methods such as submodular point processes [IB15a] and log-submodular probability distributions [DK14; DK15; DJK18], which include DPPs [KT+12]. Sampling from such distributions produces subsets that are more likely diverse than otherwise. This is often known as negative dependence where similar items have a lower probability of
being seen within the same sample than dissimilar items.

Of course, another important use for a summary is to reduce the costs and time associated with data labeling endeavors. For example, given a large unlabeled and redundant dataset, it is inefficient to label all of it. Labeling a representative summary and training on that subset, or using it in a semi-supervised learning procedure, reduces the cost and time of data labeling, not to mention that the act of labeling a diverse summary can be less susceptible to the act of labeling redundant data which can be tiresome. It is just as easy to instantiate a submodular function over unlabeled data as it is to do so over labeled data, as has been done in [Wei+14b] and which can be seen as a form of single seed-stage or batch active learning [WIB15]. More formal relationships between submodular optimization and batch active learning can be found in [GB11b] where it is shown that a form of submodular optimization selects a set that directly reduces an upper bound on the training error in a semi-supervised context.

### 3.1.6 Feature Selection

The methods above have focused on reducing the number of samples in a training dataset. Considering the transpose of a design matrix, however, all of the above methods can be used for reducing the features of a machine learning procedure as well. Specifically, any of the extractive summarization, subset selection, or coreset methods can be seen as feature selection while any of the abstract summarization, sketching, or distillation approaches can be seen as dimensionality reduction. Conversely, any strategy used for feature selection could, on principle, be used for data subset selection and any strategy used for dimensionality reduction (such as PCA, LDA, factor analysis, or even visualization methods such as tSNE or UMAP, or modified versions thereof due to the different relative sizes of \( m \) vs \( n \) in the design matrix) could be used for distillation.

### 3.2 Combinatorial Information Functions

The entropy function over a set of random variables \( X_1, X_2, \ldots, X_n \) is defined as \( H(X_1, X_2, \ldots, X_n) = -\sum_{x_1, x_2, \ldots, x_n} p(x_1, \ldots, x_n) \log p(x_1, \ldots, x_n) \). From this we can define three set-argument conditional mutual information functions as \( I_H(A; B|C) = I(X_A; X_B|X_C) \) where the latter is the mutual information between variables indexed by \( A \) and \( B \) given variables indexed by \( C \). This mutual information expresses the residual information between \( X_A \) and \( X_B \) that is not explained by their common information with \( X_C \).

As mentioned above, we may view any polymatroid function as a type of information function over subsets of \( V \). That is, \( f(A) \) is the information in set \( A \) --- to the extent that this is true, this property justifies \( f \)'s use as a summarization objective as mentioned above. The reason \( f \) may be viewed as an information function stems from \( f \) being normalized, \( f \)'s non-negativity, \( f \)'s monotonicity, and the property that further conditioning reduces valuation (i.e., \( f(A|B) \geq f(A|B, C) \) which is identical to the submodularity property). These properties were deemed as essential to the entropy function in Shannon’s original work [Sha48] but are true of any polymatroid function as well. Hence, given any polymatroid function \( f \), it is possible to define a combinatorial mutual information function [Iye+21a] in a similar way. Specifically, we can define the combinatorial (submodular) conditional mutual information (CCMI) as \( I_f(A; B|C) = f(A + C) + f(B + C) - f(C) - f(A + B + C) \), which has been known as the connectivity function [Cun83] amongst other names. If \( f \) is the entropy function, then this yields the standard entropic mutual information but here the mutual information can be defined for any submodular information measure \( f \). For an arbitrary polymatroid \( f \), therefore, \( I_f(A; B|C) \) can be seen as an \( A, B \) set-pair similarity score that ignores, neglects, or discounts any common similarity between the \( A, B \) pair that is due to \( C \).

Historical use of a special case of CCMI, i.e., \( I_f(A; B) \) where \( C = \emptyset \), occurred in a number of circumstances. For example, in [GKS05b] the function \( g(A) = I_f(A; V \setminus A) \) (which, incidentally, is both symmetric \( g(A) = g(V \setminus A) \) for all \( A \) and submodular was optimized using the greedy procedure which has a guarantee as long as \( g(A) \) is monotone up \( 2k \) elements whenever one wishes for a summary of size \( k \). This was done for \( f \) being the entropy function, but it can be used for any polymatroid function. In similar work where \( f \) is Shannon entropy, [KG05] demonstrated that \( g_C(A) = I_f(A; C) \) for a fixed set \( C \) is not submodular in \( A \) but if it is the case that the elements of \( V \) are independent given \( C \) then submodularity is preserved. This can be seen quickly by the consequence of the assumption which states that \( I_f(A; C) = f(A) - f(A|C) = f(A) - \sum_{a \in A} f(a|C) \).
where the second equality is due to the conditional independence property. In this case, $I_f$ is the difference between a submodular and a modular function which preserves submodularity for any polymatroid $f$.

On the other hand, it would be useful for $g_{B,C}(A) = I_f(A; B|C)$, where $B$ and $C$ are fixed, to be possible to optimize in terms of $A$. One can view this function as one that, when it is maximized, chooses $A$ to be similar to $B$ in a way that neglects or discounts any common similarity that $A$ and $B$ have with $C$. One option to optimize this function to utilize difference of submodular [NB05; IB12] optimization as mentioned earlier. A more recent result shows that in some cases $g_{B,C}(A)$ is still submodular in $A$. Define the second order partial derivative of a submodular function $f$ as follows $f(i, j|S) = f(j|S) - f(i|S)$. Then if it is the case that $f(i, j|S)$ is monotone non-decreasing in $S$ for $S \subseteq V \setminus \{i, j\}$ then $I_f(A; B|C)$ is submodular in $A$ for fixed $B$ and $C$. It may be thought that only isometric functions have this property but in fact [Iye+21a] shows that this is true for a number of widely used submodular functions in practice, including the facility location function which results in the form $I_f(A; B|C) = \sum_{v \in V} \max \min \{ \sum_{a \in A} \sim(v, a), \max_{b \in B} \sim(v, b) \} - \max_{c \in C} \sim(v, c)$. This function was used [Kot+22] to produce summaries $A$ that were particularly relevant to a query given by $B$ but that should neglect information in $C$ that can be considered “private” information to avoid.

Entropic quantities from the field of information theory such as entropy mutual information, conditional mutual information, and the Kullback-Leibler divergence have had an enormous impact on the field of machine learning. Each one of these measures involves at least one joint probability distribution over the set of random variables that are being measured. The submodular combinatorial measures, however, are not based on an underlying probability distribution and hence, unlike the entropic queries, are computationally more tractable. That is, even a single entropic query requires an exponential cost to exactly compute since the entropy is sum of an exponential, in the number of random variables, number of terms. While Gaussian entropy is a special case and can be computed relatively easily since it is only a log-determinant, there are many other submodular functions as we’ve seen that are easier to evaluate than even log-determinants.

### 3.3 Clustering, Data Partitioning, and Parallel Machine Learning

There are an almost limited number of clustering algorithms and a plethora of reviews on their variants. Any given submodular function can also instantiate a clustering procedure as well, and there are several ways to do this. Here we offer only a brief outline of the approach. In the last section, we defined $I_f(A; V \setminus A)$ as the CCMI between $A$ and everything but $A$. When we view this as a function of $A$, then $g(A) = I_f(A; V \setminus A)$ and $g(A)$ is a symmetric submodular function that can be minimized using Queyranne’s algorithm [Que98; NJ92]. Once this is done, the resulting $A$ is such that it is least similar to $V \setminus A$, according to $I_f(A; V \setminus A)$ and hence forms a 2-clustering. This process can then be recursively applied where we form two new functions $g_A(B) = I_f(B; A \setminus B)$ for $B \subseteq A$ and $g_{V \setminus A}(B) = I_f(B; (V \setminus A) \setminus B)$ for $B \subseteq V \setminus A$. These are two symmetric submodular functions on different ground sets that also can be minimized using Queyranne’s algorithm. This recursive bisection algorithm then repeats until the desired number of clusters is formed. Hence, the CCMI function can be used as a top-down recursive bisection clustering procedure and has been called Q-clustering [NJB05b; NB06]. It should be noted that such forms of clustering often generalize forming a multiway cut in an undirected graph in which case the objective becomes the graph-cut function that, as we saw above, is also submodular. In some cases, the number of clusters need not be specified in advance [NKI10]. Another submodular approach to clustering has already been seen in Equation 41 where the goal is to minimize the maximum valued block in a partitioning which can lead to submodular load balancing or minimum makespan scheduling [HS88; LST90] as we have seen. Also, in this light submodular fair allocation or submodular welfare can themselves be seen as a form of anti-clustering, where each block of the partition should be diverse rather than homogeneous.

Yet another form of clustering can be seen via the simple cardinality constrained submodular maximization process itself which can be compared to a $k$-medoids process whenever the objective $f$ is the facility location function. Hence, any such submodular function can be seen as a submodular-function-parameterized form of finding the $k$ ‘centers’ among a set of data items. There have been numerous applications of submodular clustering. For example, using these techniques it is possible to identify parcellations of the human brain [Sal+17]. Other applications include partitioning data for more effective and accurate and lower variance distributed machine learning training [Wei+15a] and also for more ideal mini-batch construction for training deep neural networks [Wan+19].
3.4 Active and Semi-Supervised Learning

Active learning [ACL90; CAL94; CGJ96; Set09] is a learning setting where it is acknowledged that acquiring the labels for samples is a more challenging prospect than acquiring just the unlabeled samples which can be found in abundance. Rather than impulsively and passively labeling all of your data, active learning algorithms involve iteratively and actively asking the model, as it is being learnt, which samples are most likely to be usefully labeled. This can be done in a theoretical context, where the query is done to maximally reduce a version space of possible model hypotheses [CAL94; Das05] that agree with the labels queried so far. Active learning also has many empirical and practical variants where the still unlabeled samples for which the model possesses the most uncertainty are queried first in order to reduce residual uncertainty about the remaining unlabeled samples. The critical difference between active learning is that, unlike passive learning where labels are acquired for samples regardless of how useful they might be, with active learning labels are acquired adaptively, where the next label acquired is based on the labels so far acquired, and therefore active learning has the potential to be more label efficient (i.e., more information per label) when less than 100% of the samples are labeled.

Suppose we are given data set \( \{x_i, y_i\}_{i \in V} \) consisting of \( |V| = n \) samples of \( x, y \) pairs but where the labels are unknown. Samples are labeled one at a time or one mini-batch at a time, and after each labeling step \( t \) each remaining unlabeled sample is given a score \( s_i(x_i) \) that indicates the potential benefit of acquiring a label for that sample. Examples include the entropy of the model’s output distribution on \( x_i \), or a margin-based score consisting of the difference between the top and the second-from-the-top posterior probability. This produces a modular function on the unlabeled samples, \( m_t(A) = \sum_{x \in A} s_i(x) \) where \( A \subseteq V \). It is simple to use this modular function to produce a mini-batch active learning procedure where at each stage we form \( A_t = \arg\max_{A \subseteq U_t, |A| = k} m_t(A) \) where \( U_t \) is the set of labeled samples at stage \( t \). Then \( A_t \) is a set of size \( k \) that gets labeled, we form \( U_t = U_t \setminus A_t \), update \( s_i(a) \) for \( a \in U_t \) and repeat. This is called active learning.

The reason for using active learning with mini-batches of size greater than one is that it is often inefficient to ask for a single label at a time. The problem with such a minibatch strategy, however, is that the set \( A_t \) can be redundant. The reason is that the uncertainty about every sample in \( A_t \) could be owing to the same underlying cause --- even though the model is most uncertain about samples in \( A_t \), once one sample in \( A_t \) is labeled, it may not be optimal to label the remaining samples in \( A_t \) due to this redundancy. Utilizing submodularity, therefore, can help reduce this redundancy. Suppose \( f_1(A) \) is a submodular diversity model over samples at step \( t \). At each stage, choosing the set of samples to label becomes \( A_t = \arg\max_{A \subseteq U_t, |A| = k} m_t(A) + f_1(A) \) --- \( A_t \) is selected based on a combination of both uncertainty (via \( m_t(A) \)) and diversity (via \( f_1(A) \)). This is precisely the submodular active learning approach taken in [WIB15; Kau+19]. There is other work that models uncertainty and diversity in different ways [SS18b; KAG19; Ash+20].

Another quite different approach to a form of submodular “batch” active learning setting where a batch \( L \) of labeled samples are selected all at once and then used to label the rest of the unlabeled samples. This also allows the remaining unlabeled samples to be utilized in a semi-supervised framework [GB09; GB11b]. In this setting, we start with a graph \( G = (V, E) \) where the nodes \( V \) need to be given a binary \( \{0,1\} \)-valued label, \( y \in \{0,1\}^V \). For any \( A \subseteq V \) let \( y_A \in \{0,1\}^A \) be the labels just for node set \( A \). We also define \( V(y) \subseteq V \) as \( V(y) = \{v \in V : y_v = 1\} \). Hence \( V(y) \) are the graph nodes labeled \( 1 \) by \( y \) and \( V \setminus V(y) \) are the nodes labeled \( 0 \). Given submodular objective \( f \), we form its symmetric CCMI variant \( I_f(A) = I_f(A, V \setminus A) \) --- note that \( I_f(A) \) is always submodular in \( A \). This allows \( I_f(V(y)) \) to determine the “smoothness” of a given candidate labeling \( y \). For example, if \( I_f \) is the weighted graph cut function where each weight corresponds to an affinity between the corresponding two nodes, then \( I_f(V(y)) \) would be small if \( V(y) \) (the 1-labeled nodes) do not have strong affinity with \( V \setminus V(y) \) (the 0-labeled nodes). In general, however, \( I_f \) can be any symmetric submodular function. Let \( L \subseteq V \) be any candidate set of nodes to be labeled, and define \( \Psi(L) = \min_{T \subseteq L \cup V \setminus L : \#T = |L|} I_f(T)/|T| \). Then \( \Psi(L) \) measures the “strength” of \( L \) in that if \( \Psi(L) \) is small, an adversary can label nodes other than \( L \) without being too unsmooth according to \( I_f \), while if \( \Psi(L) \) is large, an adversary can do no such thing. Then [GB11b] showed that given a node set \( L \) to be queried, and the corresponding correct labels \( y_L \) that are completed (in a semi-supervised fashion) according to the following \( y' = \arg\min_{y \in \{0,1\}^V} I_f(V(\tilde{y})) \), then this results in the following bound on the true labeling \( ||y - y'||^2 \leq 2I_f(V(y))/\Psi(L) \) suggesting that we can find a good set to query by maximizing \( L \) in \( \Psi(L) \), and this holds for any submodular function. Of course, it is necessary to find an underlying submodular function \( f \) that fits a given problem, and this is discussed in Section 3.1.
3.5 Probabilistic Modeling

Graphical models are often used to describe factorization requirements on families of probability distributions. For example, given a graph $G = (V, E)$ where the graph can be described by a set of cliques $C(G)$ where for each $C \in C(G)$ the nodes are mutually connected, it is possible to write $p(x) = \prod_{C \in C(G)} \phi_C(x_C) = 1/Z \exp(\sum_{C \in C(G)} -E_C(x_C))$ where $E(x) = \sum_{C \in C(G)} E_C(x_C)$ is a non-negative energy function and $Z$ the partition function and where, for simplicity in this section, we assume $x \in \{0, 1\}^V$ is a binary vector. Being able to discuss families of distributions all of which have this factorization property makes it possible to derive inference algorithms that work well (or approximately well) for any distribution that factors in this way according to the graph. A well-known complexity parameter associated with a graphical model is the tree-width. Performing exact probabilistic inference in a distribution that factors with respect to a graphical model has a cost that is, in the worst case, exponential in the treewidth of the corresponding graph. This is even true for MAP inference, i.e., computing $\arg\max_x p(x)$ can be exponentially costly in the tree width of the graph within whose family $p$ resides. There is a plethora of algorithms for approximate inference, many of which make additional factorization assumptions in order to achieve a given approximation [WJ08].

Factorization is not the only way, however, to describe restrictions on such families. In a graphical model, graphs describe only which random variable may directly interact with other random variables. An entirely different strategy for producing families of often-tractable probabilistic models can be produced without requiring any factorization property at all. Considering an energy function $E(x)$ where $p(x) \propto \exp(E(x))$, factorizations correspond to there being cliques in the graph such that the graph’s tree-width often is limited. On the other hand, finding $\max_x p(x)$ is the same as finding $\min_x E(x)$, something that can be done if $E(x) = f(V(x))$ is a submodular function (using the earlier used notation $V(x)$ to map from binary vectors to subsets of $V$). Even a submodular function as simple as $f(A) = \sqrt{|A|} - m(A)$ where $m$ is modular has tree-width of $n - 1$, and this leads to an energy function $E(x)$ that allows $\max_x p(x)$ to be solved in polynomial time using submodular function minimization (see Section 2.3.3). Such restrictions to $E(x)$ therefore are not of the form amongst the random variables, who is allowed to directly interact with whom, but rather amongst the random variables, what is the manner that they interact. Such potential function restrictions can also combine with direct interaction restrictions as well and this has been widely used in computer vision, leading to cases where graph-cut and graph-cut like “move making” algorithms (such as alpha-beta swap and alpha-expansion algorithms) used in attractive models [BVZ99; BK01; BVZ01b; SWW08]. In fact, the culmination of these efforts [KZ02] lead to a rediscovery of the submodularity (or the “regular” property) as being the essential ingredient for when Markov random fields can be solved using graph cut minimization, which is a special case of submodular function minimization.

The above model can be seen as log-supermodular since $\log p(x) = -E(x) + \log 1/Z$ is a supermodular function. These are all distributions that put high probability on configurations that yield small valuation by a submodular function. Therefore, these distributions have high probability when $x$ consists of a homogeneous and for this reason they are useful for computer vision segmentation problems (e.g., in a segment of an image, the nearby pixels should roughly be homogeneous as that is often what defines an object). The DPPs we saw above, however, are an example of a log-submodular probability distribution since $f(X) = \log \det(M_X)$ is submodular. These models have high probability for diverse sets.

More generally, $E(x)$ being either a submodular or supermodular function can produce log-submodular or log-supermodular distributions, covering both cases above where the partition function takes the form $Z = \sum_{A \subseteq V} \exp(f(A))$ for objective $f$. Moreover, we often wish to perform tasks much more than just finding the most probable random variable assignments. This includes marginalization, computing the partition function, constrained maximization, and so on. Unfortunately, many of these more general probabilistic inference problems do not have polynomial time solutions even though the objectives are submodular or supermodular. On the other hand, such structure has opened the doors to an assortment of new probabilistic inference procedures that exploit this structure [DK14; DK15; DTK16; ZDK15; DJK18]. Most of these methods were of the variational sort and offered bounds on the partition function $Z$, sometimes making use of the fact that submodular functions have easily computable semi-gradients [IB15b; Fuj05] which are modular upper and lower bounds on a submodular or supermodular function that are tight at one or more subsets. Given a submodular (or supermodular) function $f$ and a set $A$, it is possible to easily construct (in linear time) a modular function upper bound $m^A : 2^V \to \mathbb{R}$ and a modular function lower bound $m_A : 2^V \to \mathbb{R}$ having the properties that $m_A(X) \leq f(X) \leq m^A(X)$ for all $X \subseteq V$ and that is tight at
We have only just touched the surface of submodularity and how it can benefit machine learning. From wide and fruitful avenues for machine learning exploration. This function is convex, but it is not a norm, but if we consider the construct defined as\(\text{penalize} \) partition function, and much else.

Based upon work supported by the National Science Foundation under Grant No. 2106389. in JUMP, a Semiconductor Research Corporation (SRC) program sponsored by DARPA. This material is of convexity, therefore, the submodular inequality belies much of its complexity while opening the gates to interesting to once again revisit the innocuous looking submodular inequality. Very much like the definition of ideas and techniques in a broad way. While the above offers only a glimpse of its expressiveness, it is submodularity and the discrete optimization it entails opens up the machine learning scientist’s toolbox data summarization to clustering and active learning to parameterized sparse norms to data partitioning, 4 Conclusions

Section 3.1 can be used to produce a submodular function to instantiate an appropriate convex structured norms are used ubiquitously in machine learning, often as complexity penalizing regularizers (e.g., the ubiquitous p-norms for \(p \geq 1\)) and also sometimes as losses (e.g., squared error). Identifying new useful structured and possibly learnable sparse norms is an interesting and useful endeavor, and submodularity can help here as well. Firstly, recall the \(\ell_0\) or counting norm \(\|x\|_0\) simply counts the number of nonzero entries in \(x\). When we wish for a sparse solution, we may wish to regularize using \(\|x\|_0\) but it both leads to an intractable combinatorial optimization problem, and it leads to an object that is not differentiable. The usual approach is to find the closest convex relaxation of this norm and that is the one norm or \(\|x\|_1\). This is convex in \(x\) and has a sub-gradient structure and hence can be combined with a loss function to produce an 
norm for a given machine learning problem.

\[\|G\|_1 = \sum_{i \in G} \|w_i\|_1\]

\[5 \leq \|G\|_5\]

\[\ell[IB15b]\]

\[\text{simply counts the number of nonzero entries in } x.\]

\[\text{penalize based on its absolute value irrespective of the state of any of the other elements.}\]

\[\text{the group lasso } \|x\|_1 \text{ has no structure, as each element of } x \text{ is penalized based on its absolute value irrespective of the state of any of the other elements.}\]

\[\text{Thus, a modular approximation of a submodular function is like a mean-field approximation of the distribution and makes the assumption that all random variables are independent.}\]

\[\text{an intractable combinatorial optimization problem, and it leads to an object that is not differentiable. The usual approach is to find the closest convex relaxation of this norm and that is the one norm or } \|x\|_1.\]

\[\text{This is convex in } x \text{ and has a sub-gradient structure and hence can be combined with a loss function to produce an optimizable machine learning objective, for example the lasso. On the other hand, } \|x\|_1 \text{ has no structure, as each element of } x \text{ is penalized based on its absolute value irrespective of the state of any of the other elements.}\]

\[\text{There have thus been efforts to develop group norms that penalize groups or subsets of elements of } x \text{ together, such as group lasso } \|x\|_1.\]

\[\text{It turns out that there is a way to utilize a submodular function as the regularizer. Penalizing } x \text{ via } \|x\|_0 \text{ is identical to penalizing it via } |V(x)| \text{ and note that } m(A) = |A| \text{ is a modular function. Instead, we could penalize } x \text{ via } f(V(x)) \text{ for a submodular function } f.\]

\[\text{Here, any element of } x \text{ being non-zero would allow for a diminishing penalty of other elements of } x \text{ being zero all according to the submodular function, and such cooperative penalties can be obtained via a submodular parameterization. Like when using the zero-norm } \|x\|_0\text{, this leads to the same combinatorial problem due to continuous optimization of } x \text{ with a penalty term of the form } f(V(x)).\]

\[\text{To address this, we can use the Lovász extension mentioned above } \tilde{f}(x) \text{ on a vector } x.\]

\[\text{This function is convex, but it is not a norm, but if we consider the construct defined as } \|x\|_f = \tilde{f}(|x|), \text{ it can be shown that this satisfies all the properties of a norm for all non-trivial submodular functions } [\text{PG98; Bac+13}] \text{ (i.e., those normalized submodular functions for which } f(v) > 0 \text{ for all } v). \text{ In fact, the group lasso mentioned above is a special case for a particularly simple feature-based submodular function (a sum of min-truncated cardinality functions). But in principle, the same submodular design strategies mentioned in Section } 3.1 \text{ can be used to produce a submodular function to instantiate an appropriate convex structured norm for a given machine learning problem.}\]

4 Conclusions

We have only just touched the surface of submodularity and how it can benefit machine learning. From data summarization to clustering and active learning to parameterized sparse norms to data partitioning, submodularity and the discrete optimization it entails opens up the machine learning scientist’s toolbox of ideas and techniques in a broad way. While the above offers only a glimpse of its expressiveness, it is interesting to once again revisit the innocuous looking submodular inequality. Very much like the definition of convexity, therefore, the submodular inequality belies much of its complexity while opening the gates to wide and fruitful avenues for machine learning exploration.

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