Extended Deep Submodular Functions

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Abstract

We introduce a novel category of set functions called Extended Deep Submodular functions (EDSFs), which are neural network-representable. EDSFs serve as an extension of Deep Submodular Functions (DSFs), inheriting crucial properties from DSFs while addressing innate limitations. It is known that DSFs can represent a limiting subset of submodular functions. In contrast, through an analysis of polymatroid properties, we establish that EDSFs possess the capability to represent all monotone submodular functions, a notable enhancement compared to DSFs. Furthermore, our findings demonstrate that EDSFs can represent any monotone set function, indicating the family of EDSFs is equivalent to the family of all monotone set functions. Additionally, we prove that EDSFs maintain the concavity inherent in DSFs when the components of the input vector are non-negative real numbers—an essential feature in certain combinatorial optimization problems. Through extensive experiments, we illustrate that EDSFs exhibit significantly lower empirical generalization error than DSFs in the learning of coverage functions. This suggests that EDSFs present a promising advancement in the representation and learning of set functions with improved generalization capabilities.

1 Introduction

Submodular functions have found extensive applications in various fields of study, including modeling influence in social networks Kempe et al. (2003), energy functions in probabilistic models Gillenwater et al. (2012), and clustering Narasimhan et al. (2005). In particular in economics, a wide range of scenarios incorporate the concept of diminishing marginal return, where acquiring more goods results in diminishing the overall satisfaction or the so-called "utility" McLaughlin & Chernew (2001); Kimball et al. (2024).

There are several challenges associated with the widespread use of these functions in recent machine learning applications. To improve the modeling of submodular functions in these applications, efforts have been made to represent submodular functions using differentiable functions, such as neural networks. This representation enables the solution of key submodular optimization problems through the utilization of gradient-based methods and convex optimization. To illustrate this, suppose we want to maximize a submodular function f under certain constraints. In the exhaustive-search approach, we would have to check all 2^n subsets, which is exponential in the size of the ground set S. However, with a differentiable representation of f, we can utilize first-order information of the function, such as gradients, and project onto the constraint set to solve the optimization problem more efficiently.

There have been previous efforts to represent submodular functions using neural networks. For instance, in Bilmes & Bai (2017), the authors introduced a neural network architecture called Deep Submodular Functions (DSFs), consisting of feedforward layers with non-negative weights and normalized non-decreasing concave activation functions. Functions in this class exhibit interesting properties, such as the concavity of the function when the components of the input vector are all non-negative real numbers. By increasing the number of layers in the DSFs architecture, the family expands, indicating that there are functions in DSFs with $n + 1$ layers that are not present in DSFs with n layers. However, as stated by the authors, DSFs cannot represent all monotone submodular functions, which highly restricts their applicability to many machine learning problems.

In this paper, we introduce a novel neural network architecture, called Extended Deep Submodular Functions (EDSFs), which not only have the capability to represent any monotone submodular functions but can also represent any monotone set functions. Moreover, same as in DSFs, when the components of the input vector are all non-negative real numbers, EDSFs are concave, an important feature applicable in various combinatorial optimization settings. In addition, our experiments demonstrate that EDSFs are able to learn one of the most complicated monotone submodular functions, i.e., coverage functions, with significantly lower empirical generalization error compared to DSFs.

The rest of the paper is organized as follows: In Section 2, we formally define DSFs and state some of their important properties. In Section 3, we introduce our augmented architecture to represent all monotone (submodular) set functions and provide a proof. In Section 4, we demonstrate the superior performance of EDSFs in learning coverage functions through numerical evaluations.

1.1 Related Works

The exploration of neural networks for modeling submodular functions is relatively sparse in the existing literature. A notable contribution is the introduction of DSFs Bilmes & Bai (2017); Dolhansky & Bilmes (2016). Building on this work, the authors in Bai et al. (2018) address the maximization of DSFs under matroid constraints, using gradient-based methods to solve the optimization problem. Their work provides theoretical guarantees, establishing a suitable approximation factor given the problem's constraints. More recently, a novel architectural approach has been proposed in De & Chakrabarti (2022), which not only preserves submodularity but also extends its applicability to a more generalized form, accommodating α-submodular functions. This signifies a notable advancement in the landscape of neural network-based modeling of submodular functions, expanding the scope of potential applications and providing a platform for exploring more nuanced and versatile representations within this domain. There are other works that attempt to represent monotone set functions using neural networks. For example, in Weissteiner et al. (2021), the authors introduce a neural network architecture that represents all monotone set functions and explore their use in designing auctions.

There are also works that approach the problem of learning (submodular) set functions from different angles: The authors in Balcan & Harvey (2018) investigate submodular functions from a learning theory perspective, developing algorithms for learning these functions and establishing lower bounds on their learnability. Moreover, the authors in Feldman & Kothari (2014) attempt to approximate and learn coverage functions in polynomial time. One of the recent approaches to train and learn set functions using modern machine learning is presented in Zaheer et al. (2017), which defines the properties of permutation invariant functions and presents a set of functions encompassing all permutation invariant objective functions.

2 Background

For a ground set S, any function $f : 2^S \to \mathbb{R}$ is referred to as a set function. Below, we present the definitions of essential concepts needed for the remainder of the discussion.

Definition 2.1. (Monotone Set Function) A set function $f : 2^S \to \mathbb{R}^+$ is called a monotone set function if for any $A \subseteq B \subseteq S$ we have,

$$f(A) \leq f(B). \tag{1}$$

Definition 2.2. (Normalized Set Function) A set function $f : 2^S \to \mathbb{R}^+$ is called a normalized set function if we have,

$$f(\emptyset) = 0. \tag{2}$$

Definition 2.3. (Modular Function) A function $m : 2^S \to \mathbb{R}^+$ is called a modular function if we have,

$$\forall A \subseteq S : m(A) = \sum_{a \in A} m(a). \tag{3}$$

Now, we can formally define submodular functions as follows.

Definition 2.4. (Submodular Function) A function $f : 2^S \to \mathbb{R}$, where S is a finite set, is *submodular* if for any $A \subseteq B \subseteq S$ and $v \notin B$, we have,

$$f(A \cup v) - f(A) \geq f(B \cup v) - f(B). \tag{4}$$

In the remainder of the paper, without loss of generality, we will focus on normalized monotone set/submodular functions. If the function is not normalized, we can simply subtract the value of $f(\emptyset)$ from the function so as to make it normalized. Note that this transformation also maintains the submodularity of the function.

Definition 2.5. (Sum of Concave Composed with Modular Functions Bilmes & Bai (2017)) Assume a finite set S (*nodes* or *input features*) with cardinality n. Given a set of $m_1, m_2, \ldots, m_k$ ($m_i : 2^S \to \mathbb{R}^+$) modular functions and $\phi_1, \phi_2, \ldots, \phi_k$ ($\phi_i : \mathbb{R}^+ \to \mathbb{R}^+$) being their corresponding **non-negative**, non-decreasing, normalized (i.e., $\phi_i(0) = 0, \forall i$), concave functions, and an arbitrary modular function $m_\pm : 2^S \to \mathbb{R}^+$, the *SCMM*, $g : 2^S \to \mathbb{R}^+$, derived by these functions is defined as,

$$g(A) = \sum_{i=1}^{k} \phi_i(m_i(A)) + m_\pm(A). \tag{5}$$

Based upon recent developments, it has been discovered that the aforementioned functions given in Equation 5 exhibit inherent submodular characteristics Bilmes & Bai (2017). Looking ahead, we can view these functions as a single-layer neural networks equipped with nonlinear activation functions that exhibit concavity properties, similar to a linear mixture of inputs followed by a stepwise activation function such as ReLU (Rectified Linear Unit) after computing the overall output values.

By employing this insight, we can expand the horizons of submodular functions by leveraging them across multiple tiers. We now introduce a pivotal concept that facilitates the utilization of advanced artificial intelligence tools, specifically deep learning.

Definition 2.6. (Deep Submodular Function Bilmes & Bai (2017)) Assume we intend to define L (i.e., depth of the network) layer DSF. If $L = 1$ we use an SCMM (without last summation). Therefore, in this case we have a single-layer $n \times k$ network (with *non-negative* weights) with submodular outputs. For $L = l > 1$ we first assume the output of $l - 1$ layers as a given $n \times k$ DSF. Let's denote the output nodes of the given DSF by $B = \{\varphi_1, \varphi_2, \ldots, \varphi_k\}$. Now we want to add one layer at the end of the given DSF. We append a $k \times m$ fully connected layer with *non-negative* weights and corresponding normalized non-decreasing concave functions $\phi_1, \phi_2, \ldots, \phi_m$ for each newly added node. Then we define the outputs of the network as $C = \{\psi_1, \psi_2, \ldots, \psi_m\}$

$$\forall v \in C : \psi_v = \phi_v \left(\sum_{u \in [k]} w_{uv} \varphi_u \right) + b_v, \tag{6}$$

and $b_v \in \mathbb{R}^+$ is a bias parameter of the node. In this scheme, we have new layer added to the DSF. Therefore, we introduced a $n \times m$ DSF with $L = l$ layers. As an example, a 3-layer DSF is shown in Figure 1.

With this understanding, one can guarantee that the outcome of this architecture forms a submodular function, as it is shown in Bilmes & Bai (2017). An established finding regarding SCMMs states that any SCMM employing an arbitrary activation function can be represented as a two-layer SCMM with only the min activation function Bilmes & Bai (2017).

Despite these findings, there exist notable limitations when it comes to DSFs. While DSFs possess a range of capabilities, they are unable to encompass all submodular functions. This implies that there will always be submodular functions that cannot be represented using any number of layers in DSFs Bilmes & Bai (2017). To address this limitation, in Section 3, we extend DSFs by adding a limited number of components in the network architecture to represent all submodular functions.

In the following, we point out certain fundamental concepts in combinatorial optimization that will be employed throughout the remainder of the paper. We commence with an exploration of polymatroids.

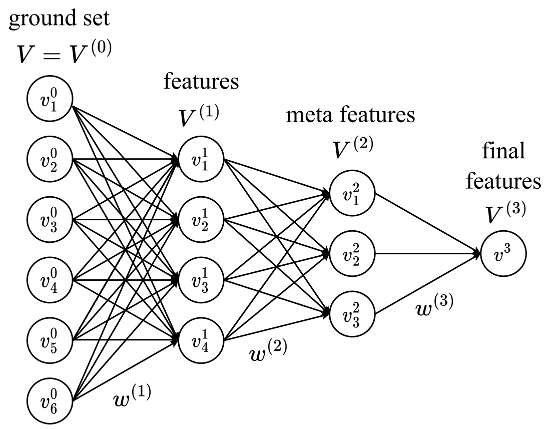


Figure 1: An example of deep submodular function Bilmes & Bai (2017).

Definition 2.7. (Polymatroid) Consider a finite set S with $|S| = s$ and a submodular function $f : 2^S \to \mathbb{R}$ defined on S. A polymatroid corresponding to f, denoted by $\mathcal{P}_f$, is defined as,

$$\mathcal{P}_f = \{\mathbf{x} \in \mathbb{R}^s : \forall A \subseteq S : \mathbf{x}(A) \leq f(A), \mathbf{x} \succeq 0\}, \tag{7}$$

where $\mathbf{x}(A) \coloneqq \sum_{i \in A} x_i$.

The following lemma describes an important property of the polymatroids corresponding to submodular functions.

Lemma 2.8. *(Goemans et al. (2009)) For a polymatroid $\mathcal{P}_f$ corresponding to a monotone submodular function f, we have*

$$\forall A \subseteq S : f(A) = \sup_{\mathbf{x} \in \mathcal{P}_f} \mathbf{x}(A). \tag{8}$$

We also define the following important submodular problem which we need later in our experiments.

Definition 2.9. (Submodular Welfare Maximization) For a collection of n users with $v_1, v_2, \ldots, v_n : 2^S \to \mathbb{R}$ as their (estimated) *submodular* valuation functions on each subset of the finite set S with $|S| = s$, the submodular welfare maximization problem aims to maximize the social welfare function, i.e., the sum of all valuation functions when we *partitioned* set of items S and assigned to the users, and is formally defined as

$$\begin{aligned} \max_{S_i, i=1,\ldots n} \quad & \sum_{i=1}^{n} v_i(S_i), \\ s.t. \quad & S_i \subseteq S, \\ & \bigcup_{i=1}^{n} S_i = S, \quad \forall i, j : S_i \cap S_j = \emptyset. \end{aligned} \tag{9}$$

Moreover, for any partition $A = \{S_1, S_2, \ldots, S_n\}$ of the ground set S to users, we define its efficiency as,

$$\mathrm{Eff}(A) \coloneqq \frac{\sum_i v_i(S_i)}{\sum_i v_i(S_i^*)} \tag{10}$$

where $OPT \coloneqq \{S_1^*, S_2^*, \ldots, S_n^*\}$ is the optimal partition.

Furthermore, in our experimental results, we will employe Coverage Functions, defined as follows.

Definition 2.10. (Coverage Function) A function $c : 2^{[n]} \to \mathbb{R}^+$ is a coverage function, if there exists a universe U with non-negative weights $w(u)$ for each $u \in U$ and subsets $A_1, A_2, \ldots, A_n$ of U such that for any $B \subseteq [n]$ we have $c(B) = \sum_{u \in \cup_{i \in B} A_i} w(u)$.

Alternatively, coverage functions can be described as non-negative linear combinations of monotone disjunctions. There are a natural subclass of submodular functions and arise in a number of applications Feldman & Kothari (2014).

3 Extended Deep Submodular Functions

3.1 Architecture Definition

Formally, we define Extended Deep Submodular Function as follows.

Definition 3.1. A set function h is an EDSF if it can be represented as the minimum of r Deep Submodular Functions $f_1, f_2, \ldots, f_r$, where r is an arbitary number, namely,

$$h(A) = \min \left\{ f_1(A), f_2(A), \ldots, f_r(A) \right\}, \quad \forall A \subseteq S. \tag{11}$$

In the rest of this section, we aim to demonstrate that we can represent any monotone submodular function f using some $g \in$ EDSFs. The idea behind the proof is to leverage the relationship between the minimum of submodular functions and the intersection of their polymatroids. The main result of this paper is summarized in the following theorem.

Theorem 3.2. *Family of monotone (submodular) set functions is exactly equal to the family of Extended Deep Submodular functions (EDSFs).*

In the following, we will go to prove this result step by step. First, we assume that a submodular function $f : 2^S \to \mathbb{R}$ is given. For convenience, we use these notations to simplify our discussion.

Definition 3.3. We define:

1. $c_A = f(A)$, and for all $j \in S$ we denote $c_j = f(\{j\})$.
2. a polytope L_A for all $A \subseteq S$ as
$$L_A = \left\{ \mathbf{x} \in \mathbb{R}^n : \mathbf{x} \succeq 0, \mathbf{x}(A) \leq c_A, \forall j \notin A : x_j \leq c_j \right\}. \tag{12}$$
3. for any $A \subseteq S$ and $B \subseteq S$ the submodular function
$$g_A(B) = \min \left\{ \sum_{j \in A \cap B} w_j, c_A \right\} + \sum_{k \in B \setminus A} w_k, \tag{13}$$
where $w_j = c_A$ for any $j \in A$ and $w_j = c_j$ for any $j \notin A$, and w_j represents the corresponding weight of some neural network.

Using these definitions, in the first step, we will show that each g_A can be represented using a simply two-layer DSF.

Lemma 3.4. *For any $A \subseteq S$, we can design a two-layer DSF that represents the g_A function, therefore the g_A function is a submodular function.*

Proof. To represent the function g_A using a DSF, we have constructed a network architecture as illustrated in Figure 2. This architecture comprises only two layers. The first layer contains two nodes, one of which employs the minimum function as its activation layer. The second layer consists of a single output node responsible for computing the sum of the inputs.

All edges connected to the lower node possess a weight of c_A. Conversely, each edge linked to the upper node bears a weight corresponding to the value c_j, specifically $f(j)$ according to the definition.

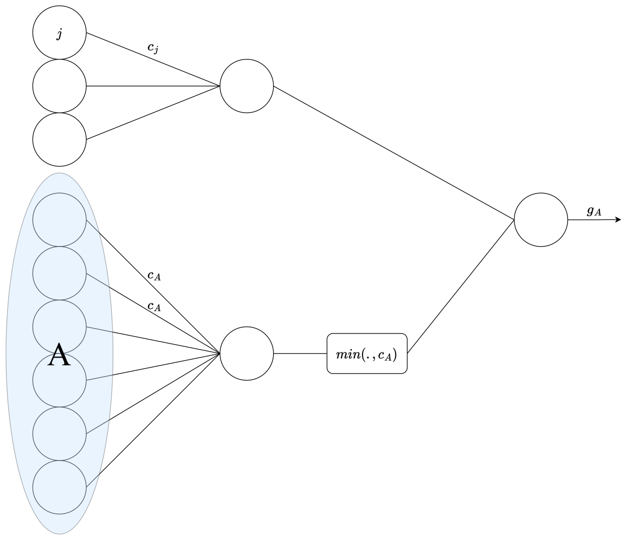


Figure 2: The simple architecture for the representation of g_A as a DSF. The function $\min(\cdot, c_A)$ is the activation function of the lower node in the hidden layer. The upper hidden node has no activation function.

In this manner, we have introduced the network as a two-layer DSF

$$g_A(B) = \min\left\{\sum_{j \in A \cap B} w_j, c_A\right\} + \sum_{k \in B \setminus A} w_k \tag{14}$$

With this, we conclude our proof. □

We next introduce a useful lemma.

Lemma 3.5. *For any $A \subseteq S$, we have*

$$\mathcal{P}_{g_A} = L_A. \tag{15}$$

Proof. To show the equality of two aforementioned sets, we first show $\mathcal{P}_{g_A} \subseteq L_A$, then we show $L_A \subseteq \mathcal{P}_{g_A}$, which completes the proof.

For the first part, for any $\mathbf{x} \in \mathcal{P}_{g_A}$, we have for all $B \subseteq S$, $\mathbf{x}(B) \leq g_A(B)$, therefore, for any $B \subseteq A$, we have $\mathbf{x}(B) \leq c_A$, in fact in this scenario $g_A(B) = 0$ or c_A, that implies $\mathbf{x}(A) \leq c_A$. Furthermore, for any $j \notin A$ we have $x_j \leq f(j) = c_j$. Therefore, each point in the polymatroid has the conditions to be in the L_A, that means, $\mathbf{x} \in L_A$.

For the reverse part, for any $\mathbf{x} \in L_A$, we have $\mathbf{x}(A) \leq c_A$, which implies that $\forall B \subseteq A, B \neq \emptyset$, $\mathbf{x}(B) \leq c_A = g_A(B)$. For any one-member subset of S, for example $B = \{j\}, j \notin A$ we have $x_j \leq c_j = g_A(B)$. Furthermore, for any arbitrary $B \subseteq S$, we could write $B = (A \cap B) \cup (B \setminus A)$. We have two cases,

1. $(A \cap B) = \emptyset$
$$\implies \mathbf{x}(B) = \sum_{j \in B \setminus A} x_j \leq \sum_{j \in B \setminus A} c_j = g_A(B)$$
2. $(A \cap B) \neq \emptyset$
$$\implies \mathbf{x}(B) = c_A + \sum_{j \in B \setminus A} x_j \leq c_A + \sum_{j \in B \setminus A} c_j = g_A(B).$$

It shows that for all $B \subseteq S$ we have: $\mathbf{x}(B) \leq g_A(B) \implies \mathbf{x} \in \mathcal{P}_{g_A}$. Therefore, the second part is now obvious, namely, $L_A \subseteq \mathcal{P}_{g_A}$. Hence,

$$\begin{cases} \mathcal{P}_{g_A} \subseteq L_A \\ L_A \subseteq \mathcal{P}_{g_A} \end{cases} \implies L_A = \mathcal{P}_{g_A}, \tag{16}$$

which completes the proof. □

For the next step, we introduce the next lemma.

Lemma 3.6. *For a given submodular function f, we have:*

$$\bigcap_{A \subseteq S} L_A = \mathcal{P}_f. \tag{17}$$

Proof. Similar to the proof of Lemma 3.5, we first show that $\bigcap_{A \subseteq S} L_A \subseteq \mathcal{P}_f$, then we will prove $\mathcal{P}_f \subseteq \bigcap_{A \subseteq S} L_A$.

For the first part, for any $\mathbf{x} \in \bigcap_{A \subseteq S} L_A$ we have

$$\forall A \subseteq S : \mathbf{x} \in L_A \implies \mathbf{x}(A) \leq c_A \implies \mathbf{x} \in \mathcal{P}_f. \tag{18}$$

Therefore, we have shown that $\bigcap_{A \subseteq S} L_A \subseteq \mathcal{P}_f$. For the reverse direction, for any $\mathbf{x} \in \mathcal{P}_f$, we can write

$$\forall A \subseteq S \implies \begin{cases} \mathbf{x}(A) \leq f(A) = c_A \\ \forall j \notin A : x_j \leq f(\{j\}) = c_j \end{cases} \implies \mathbf{x} \in L_A. \tag{19}$$

Therefore, we have shown that $\mathcal{P}_f \subseteq \bigcap_{A \subseteq S} L_A$. Combining these two parts completes our proof, namely, we have shown that $\bigcap_{A \subseteq S} L_A = \mathcal{P}_f$. □

For the next step, we need to present the following lemma.

Lemma 3.7. *For a given set $f_1, f_2, \ldots, f_r$ of submodular functions, if the function $h = \min(f_1, f_2, \ldots, f_r)$ is submodular, for the polymatroid of the function h, we have*

$$\mathcal{P}_h = \bigcap_{i=1,\ldots,r} \mathcal{P}_{f_i}. \tag{20}$$

Proof. To prove the lemma we proceed as follows.

$$\begin{aligned} \mathbf{x} \in \mathcal{P}_h &\iff \forall A \subseteq S : \mathbf{x}(A) \leq h(A) \\ &\iff \forall A \subseteq S : \forall i : \mathbf{x}(A) \leq f_i(A) \\ &\iff \forall i : \mathbf{x} \in \mathcal{P}_{f_i} \iff \mathbf{x} \in \bigcap_{i=1,\ldots,r} \mathcal{P}_{f_i}. \end{aligned}$$

□

In the next step, we introduce a new component to the DSF architecture to maintain the polymatroid corresponding to the output function to be the intersection of the polymatroids corresponding to the input functions. The proposed component is called *Min-Component*, as defined below.

Definition 3.8. (Min-Component) A Min-Component in the neural network, is a component (node) in which it brings the minimum of the inputs as the output of the node.

Incorporating this component into DSF, enhances its capability of representing submodular functions effectively.

In general, note that the min operator does not maintain the submodularity of the input functions. However, during the proof of the Theorem 3.9, we have used some techniques to assure that the output function would be submodular, as it can be seen in the following.

Moving towards the last stage, we present an architecture that is built upon the provided submodular function, as illustrated in Figure 3. In the initial layers, for any subset $A_i \subseteq S$, we have crafted the functions g_{A_i} using the architecture outlined in Figure 2. Subsequently, we applied a min-component to all of these constructed g_{A_i} functions, resulting in a composite function denoted as g. Therefore, the corresponding EDSF is generated.

In the following theorem, we establish that the function g can precisely represents the original submodular function f.

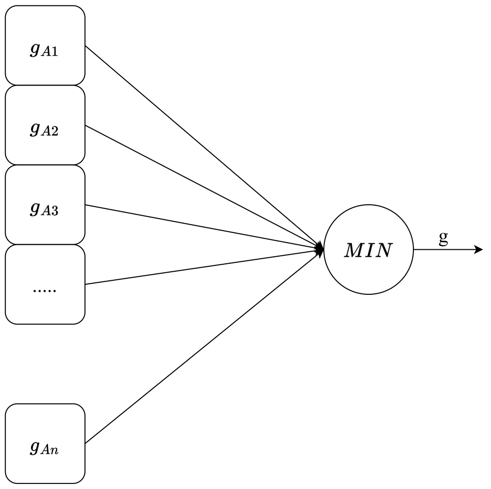


Figure 3: The architecture for the representation of the submodular function f.

Theorem 3.9. *The function g in Figure 3 exactly represents the function f. In other words*

$$\forall A \subseteq S : g(A) = f(A). \tag{21}$$

Proof. Utilizing lemmas 3.5, 3.6, and 3.7, we can deduce that the polymatroid associated with the function g is precisely identical to the polymatroid of the function f: $\mathcal{P}_g = \mathcal{P}_f$. However, it's worth noting that the function g may belong to a broader category of functions than just submodular functions.

Based on lemma 2.8, we know that there exists some $\mathbf{x}^*$ such that $\mathbf{x}^* = \underset{\mathbf{x}\in\mathcal{P}_f}{\operatorname{argmax}}\, \mathbf{x}(A)$ and $\mathbf{x}^*(A) = f(A)$. Now suppose that $f(A) > g(A)$. We can write

$$\begin{aligned} &\begin{cases} \mathbf{x}^* \in \mathcal{P} = \mathcal{P}_f = \mathcal{P}_g \\ \mathbf{x}^*(A) = f(A) \end{cases} && \implies \mathbf{x}^*(A) = f(A) > g(A) \\ & && \implies \mathbf{x}^* \notin \mathcal{P}_g \implies \mathbf{x}^* \notin \mathcal{P}_f. \end{aligned} \tag{22}$$

That is a contradiction, so for any set $A \subseteq S$ we have $g(A) \geq f(A)$.

Furthermore, we can write

$$\begin{cases} g(A) = \min_{B\subseteq S} \{g_B(A)\} \\ g_A(A) = c_A = f(A) \end{cases} \implies g(A) \leq f(A). \tag{23}$$

Combining these two results, it is clear that for any $A \subseteq S$ we have $g(A) = f(A)$. □

Up to here, we have proved that all the monotone submodular functions can be represented by an EDSF function. In the remaining of this section, we will prove that this result also holds for the family of all monotone set functions.

Lemma 3.10. *For any EDSF function f, f is monotone.*

Proof. The proof is straightforward, as all the weights used in construction of any EDSF is non-negative (all the constructing DSFs are monotone). All other functions that used in the construction of any EDSF such as min function are all monotone functions. ☐

Next we prove the final result.

Theorem 3.11. *For any monotone set function f, there exists an EDSF g, such that $f = g$.*

Proof. Consider any monotone set function f. For any $B \subseteq S$ we define g_B as follows

$$g_B(A) = \min \left\{ \sum_{j \in A \cap B} f(B), f(B) \right\} + \sum_{k \in A \setminus B} w^* \tag{24}$$

where $w^* = f(S)$, which is the maximum value function f can take (because f is monotone). Now we define function g as follows:

$$g(A) = \min_{B \subseteq S} \{g_B(A)\}. \tag{25}$$

For any $A \subseteq S$ we can see that $g_B(A) = f(A)$ if $B = A$. Now suppose $B \neq A$. If $A \setminus B \neq \emptyset$, $g_B(A) \geq f(S) \geq f(A)$, because of monotonicity. On the other hand if $A \setminus B = \emptyset$ we know that $A \subseteq B$. In this case we have $g_B(A) = f(B) \geq f(A)$, because of monotonicity. Hence we can see that $g_A(A) \leq g_B(A)$ for any $B \subseteq S$. Therefore, $g(A) = f(A)$ for all $A \subseteq S$. ☐

Based on the above results, we can conclude Theorem 3.2.

3.2 Concavity of EDSFs

We can also show that any $g \in EDSFs$ is concave, if the input vector components are all non-negative real numbers, as stated in the following theorem.

Theorem 3.12. *Given $g \in EDSFs$, g is a concave function with respect to the input vector, if the input vector components are all non-negative real numbers.*

Proof. Since all the DSF functions are concave in this setting Bilmes & Bai (2017), and g is the minimum of a number of DSFs and we know that minimum of concave functions are concave, we can conclude that g is also concave. ☐

We can exploit the above-mentioned property to solve certain combinatorial optimization problems, such as the social welfare maximization problem, using gradient-based methods in an efficient manner. This provides a powerful tool to handle some combinatorial problems. Applications in this context are discussed in Section 4.

4 Experimental Results

In the following section, we showcase a series of experiments aimed to demonstrating the positive outcomes and advantages derived from the application of Extended Deep Submodular Functions (EDSFs) in the modeling of submodular functions. Additionally, we highlight their efficacy in efficiently addressing and solving various combinatorial optimization problems. Through these experiments, we aim to provide a clear and comprehensive understanding of how EDSFs contribute to improved outcomes in the domain of submodular function modeling and the optimization of complex combinatorial scenarios.

4.1 Learning Coverage Functions

As outlined in Section 2, coverage functions constitute a crucial and intricate subset of monotone submodular functions, posing challenges in accurate learning from their instances.

Our experimental findings indicate that, in contrast to Deep Submodular Functions (DSFs), Extended Deep Submodular Functions (EDSFs) shown to be effective in efficiently learning these complex functions, exhibiting much lower empirical generalization error, compared to DSFs.

To perform the experiment, from each coverage function (defined in Definition 2.10), we generate a random dataset $\mathcal{D} = (X_i, y_i)_{i=1}^{d}$ where X_i is a random subset from the ground set S, and y_i is the value of the coverage function. In our experimental setup, we created three coverage functions with a universe size of 100 and 16 subsets. For each coverage function, we employed a Bernoulli random variable with probabilities of 0.1, 0.3, and 0.5, respectively, determining the likelihood of each item in the universe belonging to each subset independently. The weights function in the coverage function remains constant with a value of 1. We generated a dataset comprising 1024 samples, allocating 80% for training and 20% for testing.

We utilized quite similar architectures to train both Deep Submodular Functions (DSFs) and Extended Deep Submodular Functions (EDSFs) on the datasets, employing the $L1$-loss function. Subsequently, we calculated their respective empirical generalization errors on the corresponding test sets.

Notably, the training of DSFs on the above scenario proved to be unsuccessful, with the output remaining constant, likely due to the complexity of the coverage function. In contrast, EDSFs exhibited robust generalization with low error, showcasing their superior performance in this experimental context.

We report our final $L1$-loss, averaged on 100 different experiments using DSFs and EDSFs in Table 1. The details of this experiment is elaborated in Appendix A.

Coverage Prob.	Training Loss (EDSF)	Test Loss (EDSF)	Training Loss (DSF)	Test Loss (DSF)
0.1	1.0984	1.1127	25.0797	25.9907
0.3	1.0771	1.0913	13.3646	14.3648
0.5	0.6747	0.9852	6.2945	6.8395

Table 1: Training and Test $L1$-loss for EDSF and DSF setting.

Moreover, we conducted a series of experiments with different values of r, number of DSF used before using the min function, to show the effect of the size of the EDSF network on the generalization error of the training. In Table 2, we have shown the test loss for various size of r, using the same setting we discussed earlier.

We also conducted some experiments of learning coverage function with universe size of 1000, probability of 0.2, and item numbers of 50 (much larger universe size and more items, compared to the previous experiment). Firstly, we kept the same architecture for both EDSFs and DSFs and ran 20 different experiments, which the average results are shown in Table 3.

For another set of experiments, we tried different architectures for DSFs, and the result of the training is also much worse than the above EDSF's result, as can be observed below.

1. 5 hidden layers with 64 neurons each, alpha set to 95: test loss is 84.3058
2. 4 hidden layers with 64 neurons each, alpha set to 125: test loss is 84.7727
3. 5 hidden layers with respectively 32, 64, 128, 64, and 32 neurons, alpha set to 400: test loss is 81.4188

The above experimental results demonstrate the superiority of EDSF compared to DSF in learning the coverage functions.

r	Test Loss
1	82.1343
2	82.1319
4	81.9668
8	81.7255
16	3.3907
32	4.0554
64	3.1114
128	3.5768
256	16.1887
512	5.9880
1024	8.9269

Table 2: Experiments for various size of EDSF in learning coverage functions. Here, r is the number of DSF functions used in constructing the EDSF.

Arch.	Test Loss Mean	Test Loss Std.
EDSF	5.33770	1.3630
DSF	82.58076	9.0195

Table 3: Experiments for comparison of EDSF and DSF for learning coverage functions with a large universe of size 1000.

4.2 Learning Cut Functions

We conducted several experiments to learn modified graph cut functions (we choose modified version to maintain the monotonicity), which is a well-known submodular function. Firstly, we generated the random graph using Erdos-Renyi model (with probability 0.2 and 50 vertices), then, for any set of vertices X, we considered the function $f(X) = |\text{cut}(X)| + \sum_{a \in X} \deg(a)$ which is a monotone submodular function. To learn the cut function, we have used the EDSF architecture with 64 DSFs as its backbone. The result is that for 12 trials, we have (mean, standard deviation) of test loss: (4.6309, 0.5857). The additional figures are presented in Appendix B. Our experiments also demonstrated that in this particular scenario, DSFs also perform reasonably in learning cut functions.

4.3 Social Welfare Maximization

In this experiment, we leveraged the previously discussed concave property inherent in EDSFs to address the widely recognized combinatorial optimization problem of maximizing social welfare, as delineated in Section 2. In this specific context, each of the valuation functions, denoted as $v_1, v_2, \ldots, v_n$, is assumed to be an EDSF or a DSF, acquired through learning from samples collected from users. Our optimization problem, expressed in Equation 9, can be reformulated as follows,

$$\begin{aligned} \max_{a} \quad & SW(a) \triangleq \sum_{i=1}^{n} v_i(a_i), \\ s.t. \quad & \sum_{i=1}^{n} a_{ij} = 1, \text{for all} \quad j \in S, \\ & a_{ij} \in \{0,1\}. \end{aligned} \tag{26}$$

where a is a $n \times m$ matrix, such that $a_{ij} \in \{0,1\}$ meaning if item j assigned to user i and a_i represents the i'th row of a, which is the items that were assigned to user i.

Algorithm 1 Gradient Ascent

```
Input: valuation functions $v_1, v_2, \dots, v_n$, set of items $S$ ($|S| = s$), learning rate $\eta$
Initialize $a = (0)_{ij}$
Project each column of $a$ on the probability simplex
repeat
    Compute gradient of $SW$ function in the point $a = g \in \partial SW$.
    $a = a + \eta.g$
    Project each column of $a$ on the probability simplex
until convergence
for $i$ in $S$ do
    Select the user assigned to item $i$ by sampling from $i$'th column of $a$ (corresponding distribution for item $i$).
end for
```

To solve this optimization problem, first we relax it to the following form,

$$\begin{aligned} \max_{a} \quad & SW(a) = \sum_{i=1}^{n} v_i(a_i), \\ s.t. \quad & \sum_{i=1}^{n} a_{ij} = 1, \text{for all} \quad j \in S, \\ & a_{ij} \in [0, 1]. \end{aligned} \tag{27}$$

As we mentioned, each of the v_i's are EDSF or DSF, so they are concave, hence, the relaxed problem is clearly a convex problem, e.g., maximizing a concave function with convex constraints, and can be solved using convex optimization techniques such as projected gradient ascent. The projection step consists of m distinct projections on probability simplex for each item. The algorithm pseudo-code is shown in Algorithm 1.

In this experiment, we initially presumed that the true submodular value functions were Coverage Functions. Subsequently, we trained both Extended Deep Submodular Functions (EDSFs) and Deep Submodular Functions (DSFs) using pre-defined architectures for each user valuation function. We then employed gradient ascent on the social welfare function to find semi-optimal item assignment.

Exp. No.	Predicted Social Welfare	Optimal Social Welfare	Efficiency %
1	124	127	97.6378
2	114	123	92.6829
3	84	129	65.1163
4	118	128	92.1875
5	114	127	89.7638
6	126	128	98.4375
7	110	122	90.1639
8	123	132	93.1818
9	123	128	96.0938
10	120	129	93.0233
Average	115.6	127.3	90.8288

Table 4: Experiments when value functions are coverage functions, with 50 universe size, and 8 items, with probablities 0.1, 0.3, and 0.5 for three bidders respectively, and the learning model is EDSF.

Furthermore, we conducted a new experiment to compare the performance of vanilla nerual networks versus EDSFs. The results are shown in Table 6. We can see that the mean efficiency is about 77%, which is much

Exp. No.	Predicted Social Welfare	Optimal Social Welfare	Efficiency %
1	98	127	77.1654
2	98	121	80.9917
3	63	130	48.4615
4	50	124	40.3226
5	94	120	78.3333
6	92	131	70.2290
7	92	126	73.0159
8	99	129	76.7442
9	94	127	74.0157
10	60	125	48.0000
Average	84	126	66.7279

Table 5: Experiments when value functions are coverage functions, with 50 universe size, and 8 items, with probablities 0.1, 0.3, and 0.5 for three bidders respectively, and the learning model is DSF.

lower than the EDSF efficiency (90%). Also, we have conducted experiments for universe size 500 and 8 sets (items) of the coverage function. The Table 7 shows the results. Finally, we conducted experiments for universe size 1000 and 8 sets (items) for the coverage function. The Table 8 shows the results about efficiency of the algorithms.

Exp. No.	Predicted Social Welfare	Optimal Social Welfare	Efficiency %
1	56.0	98.0	57.14
2	79.0	101.0	78.28
3	89.0	93.0	95.70
4	81.0	94.0	86.17
5	70.0	99.0	70.71
6	52.0	94.0	55.32
7	84.0	100.0	84.00
8	62.0	101.0	61.39
9	88.0	99.0	88.89
10	81.0	96.0	84.37
11	77.0	93.0	82.80
12	92.0	108.0	85.19
13	77.0	104.0	74.04
14	85.0	99.0	85.86
15	69.0	94.0	73.40

Table 6: Experiments when value functions are coverage functions, with 50 universe size, and 8 items, with probablities 0.1, 0.3, and 0.5 for three bidders respectively, and the learning model is vanilla neural network.

Observing the results, it becomes apparent that the utilization of Extended Deep Submodular Functions (EDSFs) in the context of the social welfare maximization problem yields significantly higher efficiency when compared to Deep Submodular Functions (DSFs) and also vanilla neural networks. This stark difference in efficiency underscores the potential advantages and superior performance that our proposed framework, leveraging EDSFs, can bring to the modeling of user valuations within the realm of this NP-hard combinatorial optimization problem.

Exp. No.	EDSF Predicted Social Welfare	DSF Predicted Social Welfare	Optimal Social Welfare	EDSF Eff. %	DSF Eff. %
1	892.0	653.0	902.0	98.89	72.39
2	907.0	634.0	917.0	98.91	69.14
3	887.0	636.0	892.0	99.44	71.30
4	882.0	500.0	900.0	98.00	55.56
5	909.0	670.0	913.0	99.56	73.38
Average	894.0	618.0	904.0	98.96	68.35

Table 7: Experiments comparing EDSF and DSF efficiency in the maximizing social welfare problem, with coverage function as value function, 500 universe size, with probabilities 0.1, 0.3, and 0.5 for three bidders, respectively.

Exp. No.	EDSF Predicted Social Welfare	DSF Predicted Social Welfare	Optimal Social Welfare	EDSF Eff. %	DSF Eff. %
1	1737.0	1527.0	1782.0	97.47	85.69
2	1742.0	1730.0	1789.0	97.37	96.70
3	1744.0	1547.0	1778.0	98.09	87.01
4	1784.0	1739.0	1790.0	99.66	97.15
5	1755.0	1699.0	1776.0	98.82	95.66
Average	1752.4	1648.4	1783.0	98.2	92.60

Table 8: Experiments comparing EDSF and DSF efficiency in the maximizing social welfare problem, with coverage function as value function, 1000 universe size, with probabilities 0.1, 0.3, and 0.5 for three bidders, respectively.

5 Discussion

In this paper, we introduced an architecture to represent all monotone set/submodular functions using neural networks. Here are some points about the proposed architecture that are worth-noting. The most important shortcoming of this architecture is the exponential size of the network to represent all monotone set/submodular functions. However, we would like to note that the assumption on the exponentiality of the number of DSFs is just used as a sufficient condition for our proofs. In our experiments, we observed that using much less number of DSFs than exponential order is enough to attain good generalization in practice. For example, in the problem of learning coverage functions, we used 64 DSFs to represent a function with 16 and 50 items as input (note that $64 \ll 2^{16}$ and $64 \ll 2^{50}$). We have also used 64 DSFs in learning cut functions of graphs with 50 vertices ($64 \ll 2^{50}$).

On the other hand, there exist some approximation algorithm to find the near-optimal social welfare in the problem setting mentioned above, like the one proposed in Vondrak (2008), namely, Randomized or Continuous Greedy. We have conducted multiple experiments in order to compare the Continuous Greedy and Gradient Ascent algorithm as follows. We performed 20 trials with 16 items, in the setting of 3 participants with coverage functions as valuation functions that have a universe size of 1000, and various probabilities. The mean of (Gradient Ascent, Continuous Greedy) over multiple trials to find maximum social welfare is (2333.45, 2332.2). As can be seen from the results, the "average" performance of both methods (Gradient Ascent and Continuous Greedy) is very similar, leading us to conclude that there may be a shared intuition underlying both algorithms. The intuition behind the continuous greedy algorithm is that the current distribution will shift towards the most increasing direction to find the optimal distribution for sampling. This concept is reminiscent of moving in the direction of the gradient in concave functions to maximize them. Overall, it appears that the Gradient Ascent algorithm closely resembles the continuous dual of the continuous greedy algorithm. Exploring the theoretical connection between Gradient Ascent and Continuous Greedy can be an interesting direction for future work.

However, in the following, we would like to mention that the continuous greedy algorithm has two major limitations.

1. In every step, the Continuous Greedy (CG) algorithm needs to sample a large number of function calculations ($O((mn)^5)$) to determine the expected marginal increment. Moreover, it needs at least $O((mn)^2)$ steps to obtain the result. This imposes a significant computational burden on CG compared to Gradient Ascent (GA), where the gradient is calculated with much less computational complexity, since the computation of gradient is $O(1)$. This fact limits the scalability of the Continuous Greedy algorithm. we also conducted some experiments for 100 items and the GA algorithm is much faster than CG algorithm in practice.
2. Furthermore, the proposed approach is applicable to both monotone submodular and non-submodular functions, while CG is only applicable to submodular functions.

6 Conclusions

In this research, we introduce a novel concept called Extended Deep Submodular Functions (EDSFs), building upon the foundation of Deep Submodular Functions (DSFs). DSFs, a subset of monotone submodular functions, provide a structured framework for representing specific types (a subset) of submodular functions. However, the scope of DSFs is limited to a strict subset of monotone submodular functions. EDSFs, on the other hand, serve as a natural extension, expanding the family of DSFs to encompass all monotone set/submodular functions. Our proofs are rooted in the properties of polymatroids, offering insights into the relationship between polymatroids and submodular functions. Additionally, we highlight the concave nature of EDSFs, a characteristic that is proved to be valuable in addressing and efficiently solving various combinatorial optimization problems. To validate the efficacy of EDSFs, we conducted experiments in three distinct settings, namely, learning coverage functions, learning modified cut functions, and maximizing social welfare. The results consistently demonstrated the superior performance of EDSFs compared to DSFs in these experimental scenarios. In conclusion, our findings suggest that EDSFs provide a more comprehensive and effective solution for modeling monotone set/submodular functions using neural networks. The extended scope and enhanced performance make EDSFs a promising direction for further exploration in various machine learning and optimization domains.

Broader Impact

This paper presents work whose goal is to advance the field of Machine Learning. There aren't many straight potential societal consequences of our work, none which we feel must be specifically highlighted here.

References

Wenruo Bai, William Stafford Noble, and Jeff A Bilmes. Submodular Maximization via Gradient Ascent: The Case of Deep Submodular Functions. In *Advances in Neural Information Processing Systems*, volume 31. Curran Associates, Inc., 2018. URL `https://proceedings.neurips.cc/paper_files/paper/2018/hash/b43a6403c17870707ca3c44984a2da22-Abstract.html`.

Maria-Florina Balcan and Nicholas J. A. Harvey. Submodular Functions: Learnability, Structure, and Optimization. *SIAM Journal on Computing*, 47(3):703–754, January 2018. ISSN 0097-5397, 1095-7111. doi: 10.1137/120888909. URL `https://epubs.siam.org/doi/10.1137/120888909`.

Jeffrey Bilmes and Wenruo Bai. Deep Submodular Functions, January 2017. URL `http://arxiv.org/abs/1701.08939`. arXiv:1701.08939 [cs].

Abir De and Soumen Chakrabarti. Neural Estimation of Submodular Functions with Applications to Differentiable Subset Selection. 2022.

Brian W Dolhansky and Jeff A Bilmes. Deep submodular functions: Definitions and learning. *Advances in Neural Information Processing Systems*, 29, 2016.

Vitaly Feldman and Pravesh Kothari. Learning coverage functions and private release of marginals. In *Conference on Learning Theory*, pp. 679–702. PMLR, 2014. URL `https://proceedings.mlr.press/v35/feldman14a.html`.

Jennifer Gillenwater, Alex Kulesza, and Ben Taskar. Near-optimal map inference for determinantal point processes. *Advances in Neural Information Processing Systems*, 25, 2012.

Michel X. Goemans, Nicholas J. A. Harvey, Satoru Iwata, and Vahab Mirrokni. Approximating Submodular Functions Everywhere. In *Proceedings of the Twentieth Annual ACM-SIAM Symposium on Discrete Algorithms*, pp. 535–544. Society for Industrial and Applied Mathematics, January 2009. ISBN 978-0-89871-680-1 978-1-61197-306-8. doi: 10.1137/1.9781611973068.59. URL `https://epubs.siam.org/doi/10.1137/1.9781611973068.59`.

David Kempe, Jon Kleinberg, and Éva Tardos. Maximizing the spread of influence through a social network. In *Proceedings of the ninth ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 137–146, 2003.

Miles S Kimball, Daniel Reck, Fudong Zhang, Fumio Ohtake, and Yoshiro Tsutsui. Diminishing marginal utility revisited. Technical report, National Bureau of Economic Research, 2024.

CG McLaughlin and ME Chernew. Health insurance: economic and risk aspects. 2001.

Mukund Narasimhan, Nebojsa Jojic, and Jeff A Bilmes. Q-clustering. *Advances in Neural Information Processing Systems*, 18, 2005.

Jan Vondrak. Optimal approximation for the submodular welfare problem in the value oracle model. In *Proceedings of the fortieth annual ACM symposium on Theory of computing*, pp. 67–74, Victoria British Columbia Canada, May 2008. ACM. ISBN 978-1-60558-047-0. doi: 10.1145/1374376.1374389. URL `https://dl.acm.org/doi/10.1145/1374376.1374389`.

Jakob Weissteiner, Jakob Heiss, Julien Siems, and Sven Seuken. Monotone-value neural networks: Exploiting preference monotonicity in combinatorial assignment. *arXiv preprint arXiv:2109.15117*, 2021.

Manzil Zaheer, Satwik Kottur, Siamak Ravanbakhsh, Barnabas Poczos, Russ R Salakhutdinov, and Alexander J Smola. Deep sets. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett (eds.), *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017. URL `https://proceedings.neurips.cc/paper_files/paper/2017/file/f22e4747da1aa27e363d86d40ff442fe-Paper.pdf`.

A Details of Experiments on Learning Coverage Functions

In the following experiments, we trained EDSFs and DSFs with similar architectures, except the min-component at the end of the EDSFs, consists of three fully-connected layers with 64 neurons stacked with $\phi(x) = \min(\alpha, x)$, i.e., minimum linear unit, with $\alpha = 95$ as an activation function.

We have run each architecture for three distinct coverage functions described earlier in Section 4, and we have shown EDSFs has much lower empirical generalization error than DSFs. We illustrated this by providing a few samples' results, shown in Figures 4-9. These figures represent the output of experiments conducted on generated data from each coverage function for EDSFs and DSFs separately. In each run we trained the above-mentioned neural networks on the data for 10000 epochs. As it can be seen, in EDSF experiments the predicted values completely follows the true values of the coverage function.

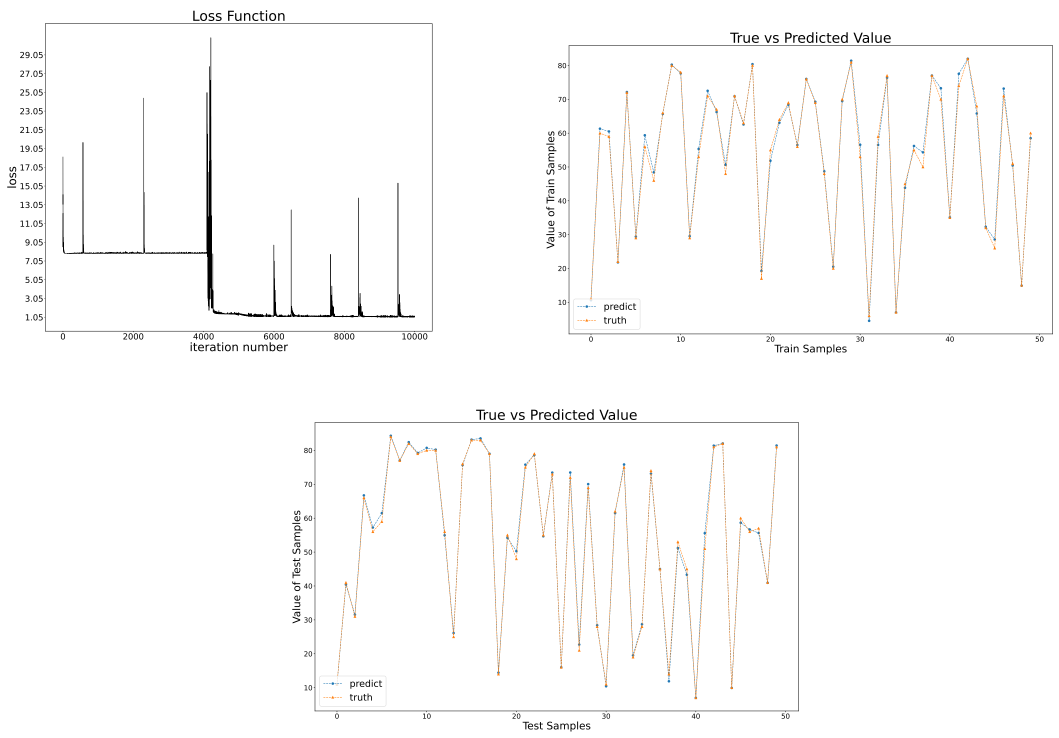
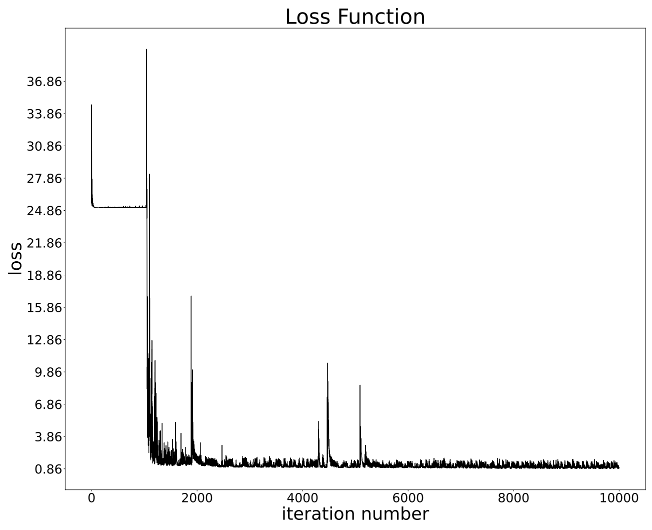
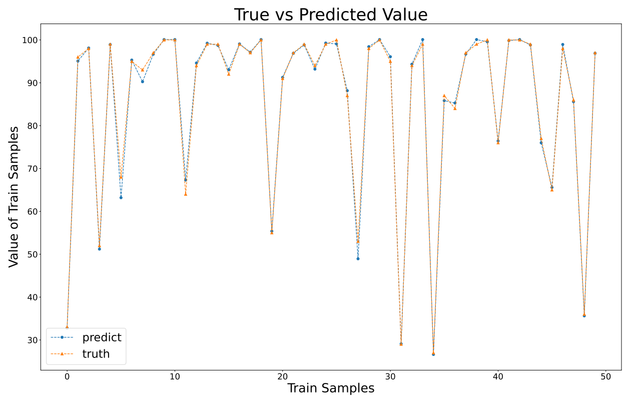


Figure 4: Learning coverage function with coverage probability 0.1, using the EDSF architecture, showing Training loss, Truth vs. Predicted values for train and test samples

B Details of Experiments on Learning Cut Functions

In the learning cut function experiment, we have used the same architecture as the one used for learning coverage functions in Appendix A. We have presented the corresponding loss and generalization error for learning cut functions in the Figure 10.





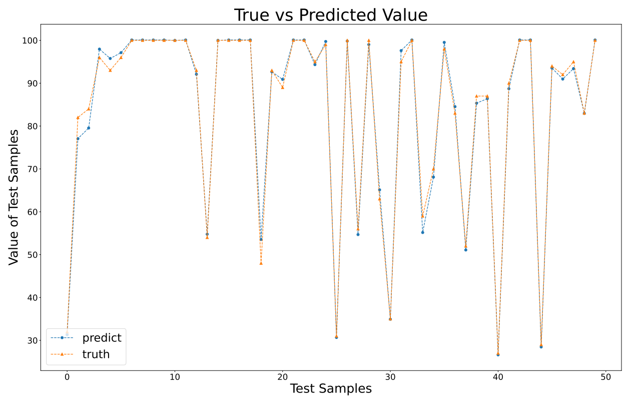
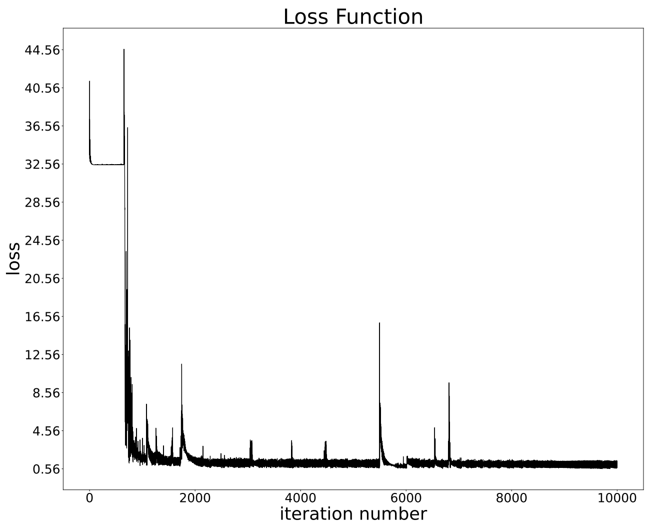
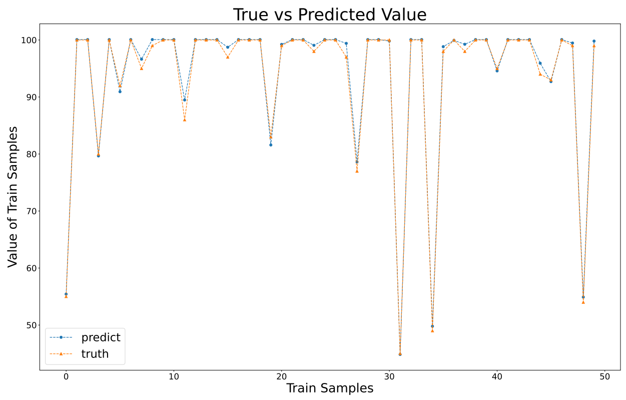


Figure 5: Learning coverage function with coverage probability 0.3, using the EDSF architecture, showing Training loss, Truth vs. Predicted values for train and test samples





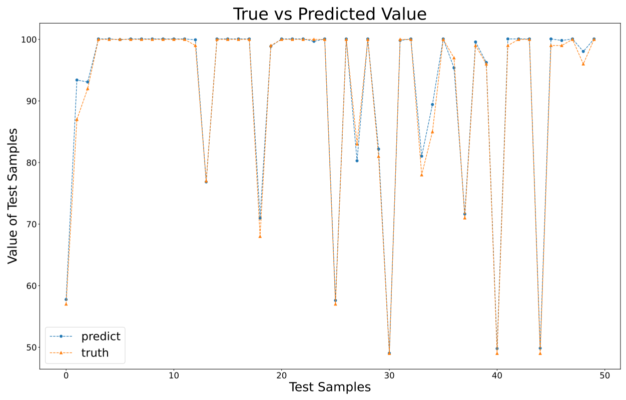
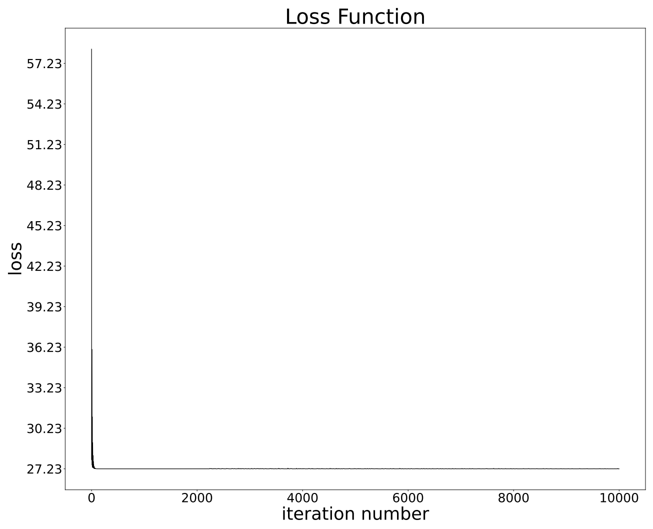
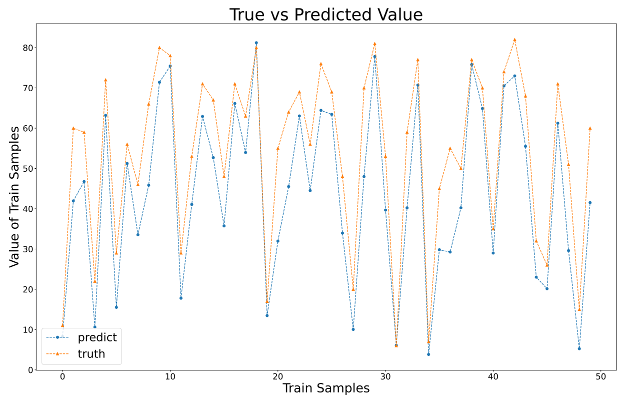


Figure 6: Learning coverage function with coverage probability 0.5, using the EDSF architecture, showing Training loss, Truth vs. Predicted values for train and test samples





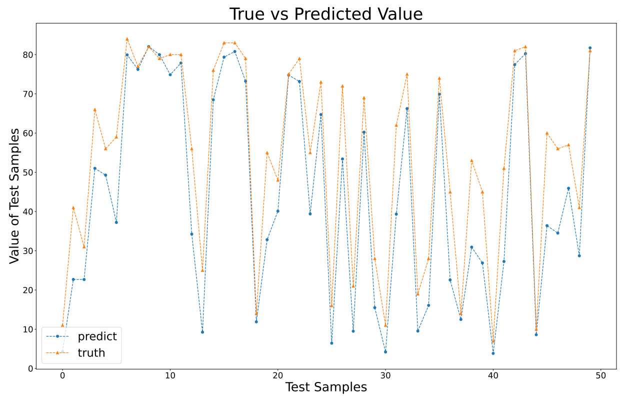
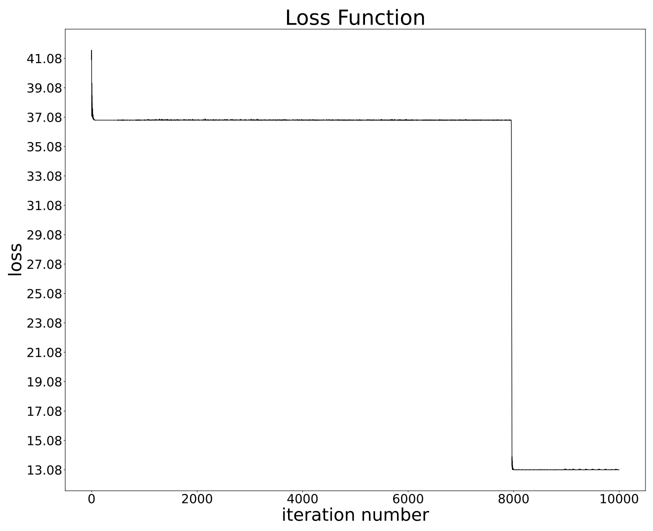
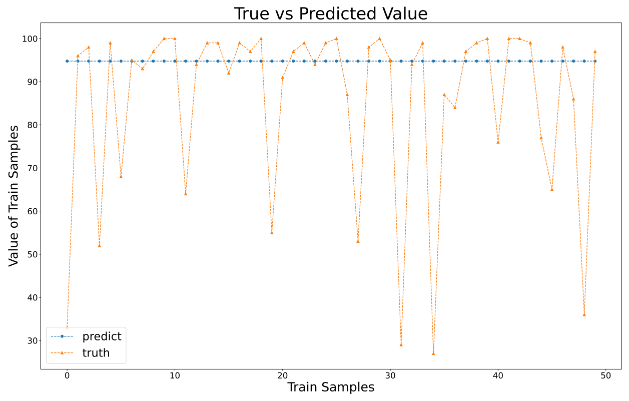


Figure 7: Learning coverage function with coverage probability 0.1, using the DSF architecture, showing Training loss, Truth vs. Predicted values for train and test samples





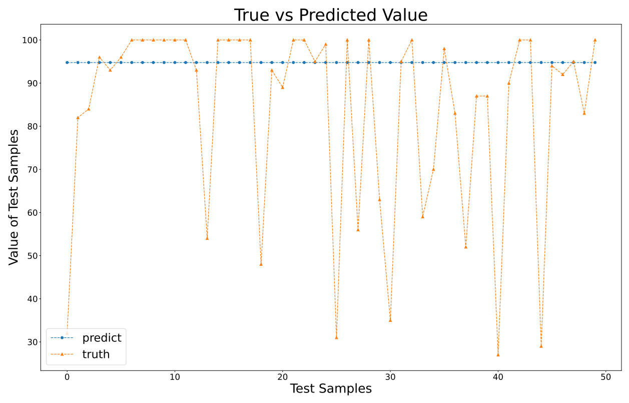


Figure 8: Learning coverage function with coverage probability 0.3, using the DSF architecture, showing Training loss, Truth vs. Predicted values for train and test samples

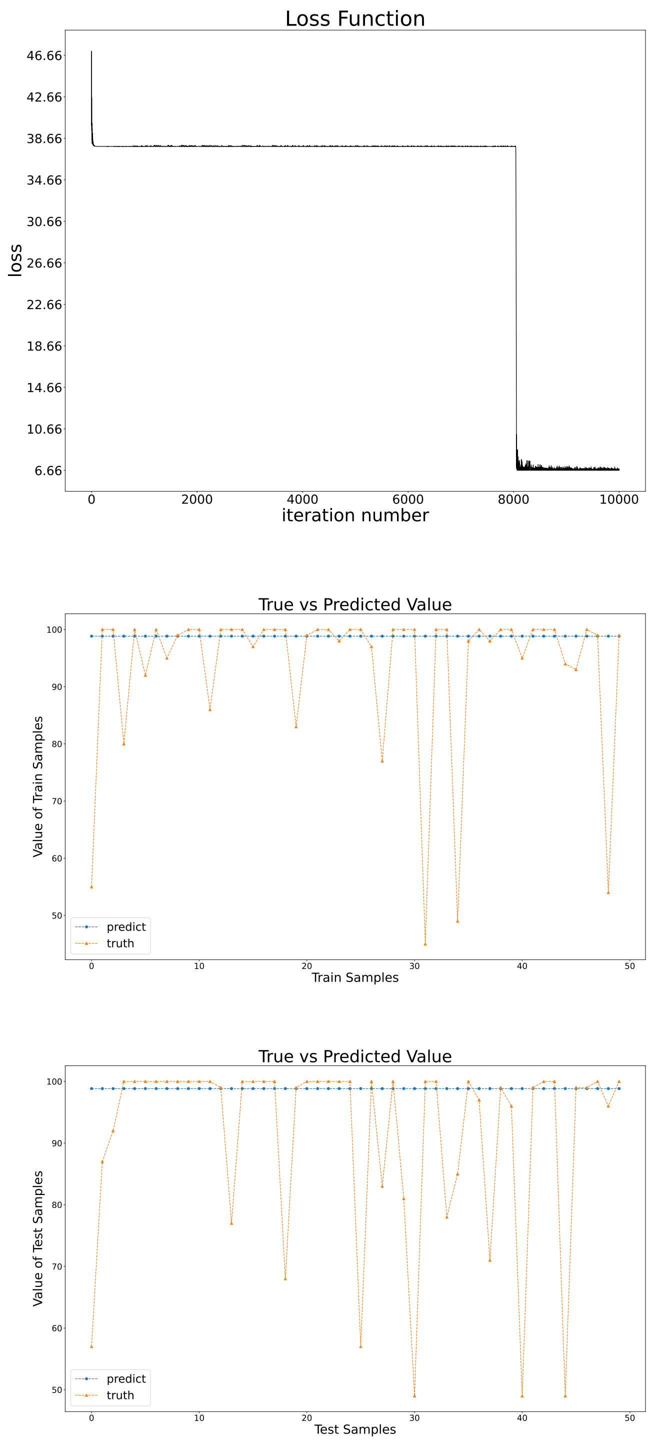


Figure 9: Learning coverage function with coverage probability 0.5, using the DSF architecture, showing Training loss, Truth vs. Predicted values for train and test samples

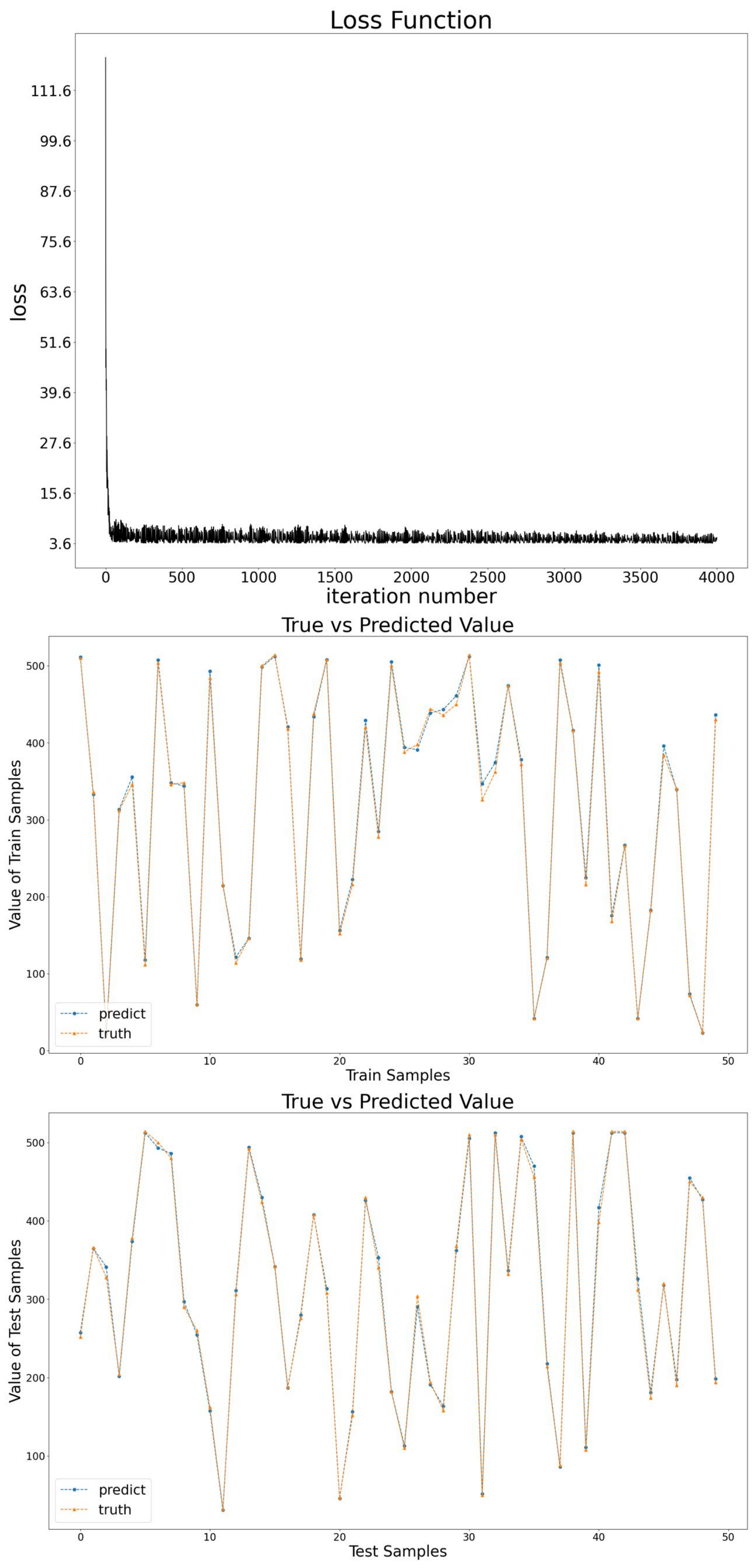


Figure 10: Learning a cut function generated by the Erdos-Renyi model with probability 0.2 and having 50 vertices, using the EDSF architecture, showing Training loss, Truth vs. Predicted values for train and test samples.