Finding the Submodularity Hidden in Symmetric Difference

Junpei Nakashima*  Yukiko Yamauchi*  Shuji Kijima†  Masafumi Yamashita*

December 27, 2017

Abstract

A fundamental property of convex functions in continuous space is that the convexity is preserved under affine transformations. A set function $f$ on a finite set $V$ is submodular if $f(X) + f(Y) \geq f(X \cup Y) - f(X \cap Y)$ for any pair $X, Y \subseteq V$. The symmetric difference transformation (SD-transformation) of $f$ by a canonical set $S \subseteq V$ is a set function $g$ given by $g(X) = f(X \triangle S)$ for $X \subseteq V$, where $X \triangle S = (X \setminus S) \cup (S \setminus X)$ is the symmetric difference between $X$ and $S$. Despite that submodular functions and SD-transformations are regarded as counterparts of convex functions and affine transformations in finite discrete space, not all SD-transformations do not preserve the submodularity. Starting with a characterization of SD-transformations that preserve the submodularity, this paper investigates the problem of discovering a canonical set $S$, given the SD-transformation $g$ of a submodular function $f$ by $S$, provided that $g(X)$ is given by an oracle. A submodular function $f$ on $V$ is said to be strict if $f(X) + f(Y) > f(X \cup Y) - f(X \cap Y)$ holds whenever both $X \setminus Y$ and $Y \setminus X$ are nonempty. We show that the problem is solvable by using $O(|V|)$ oracle calls when $f$ is strictly submodular, although it requires exponentially many oracle calls in general.

Keywords: Submodular functions, symmetric difference

1 Introduction

1.1 Submodular function and convexity

Submodular function on a finite set. For a set function $f: \{0, 1\}^V \to \mathbb{R}$ on a finite set $V$, we define

$$
\Phi_f(X,Y) \overset{\text{def.}}{=} f(X) + f(Y) - f(X \cup Y) - f(X \cap Y)
$$

(1)

for any $X, Y \subseteq V$, for convenience of the arguments of the paper. A set function $f$ is submodular if $\Phi_f(X,Y) \geq 0$ holds for any pair $X, Y \in \{0, 1\}^V$. In this paper, we do not assume $f(\emptyset) = 0$ for a submodular function $f$, which is often assumed in the literature, but this is not essential to the arguments of the paper. Similarly, a set function is modular if $\Phi_f(X,Y) = 0$ holds for any pair $X, Y \in \{0, 1\}^V$. A set function is strictly submodular if $\Phi_f(X,Y) > 0$ holds for any nontrivial pair $X, Y \in \{0, 1\}^V$, which satisfies both $X \setminus Y$ and $Y \setminus X$ are nonempty.

Submodular function is an important concept particularly in the context of combinatorial optimization, and has many applications in economics, machine learning, etc. It is well-known that minimizing a submodular function given as its function value oracle is solved efficiently, by calling the value oracle (strongly) polynomial times [17][9][10][12]. In contrast, maximizing submodular function, e.g., max cut, is NP-hard, and approximation algorithms have been developed e.g.,[15][4].

*Graduate School of Information Science and Electronic Engineering, Kyushu University
†JST PRESTO, 744 Motooka, Nishi-ku, Fukuoka, 819-0395, Japan

1 Clearly, the condition $\Phi_f(X,Y) \geq 0$ is equivalent to $f(X) + f(Y) \geq f(X \cup Y) + f(X \cap Y)$, which is often used.
A celebrated characterization of a submodular function is described by the Lovász extension (see e.g., [12], [13]). For a set function \(f: \{0,1\}^V \rightarrow \mathbb{R}\), the Lovász extension \(\hat{f}: \mathbb{R}^V \rightarrow \mathbb{R}\) is defined for \(x = (x(v)) \in \mathbb{R}^V\) which satisfies \(x(v_1) \geq x(v_2) \geq \cdots \geq x(v_{|V|})\) by \(\hat{f}(x) \overset{\text{def.}}{=} \sum_{i=1}^{|V|} x(v_i)(f(\{v_j \mid j \leq i\}) - f(\{v_j \mid j \leq i-1\})) + f(\emptyset)\). Lovász [13] showed that a set function \(f\) is submodular if and only if \(\hat{f}\) is a convex function. There are many other arguments to regard submodular functions as a discrete analogy of convex functions see e.g., [13], [14].

**Convex function in continuous space.** A function \(f: \mathbb{R}^n \rightarrow \mathbb{R}\) in a continuous space is convex if \(\lambda f(x) + (1 - \lambda)f(y) \leq f(\lambda x + (1 - \lambda)y)\) holds for any \(x, y \in \mathbb{R}^n\) and \(\lambda \in [0,1]\) (see e.g., [14]). An important property of a convex function (even on a convex set) is that local minimality guarantees the global minimality, and the convexity is regarded as tractable and useful class in the context of optimization.

As another property, the convexity is invariant under an affine map; Let \(h: \mathbb{R}^n \rightarrow \mathbb{R}^n\) be an affine map given by \(h(x) \overset{\text{def.}}{=} Ax + b\) with some \(A \in \mathbb{R}^{n \times n}\) and \(b \in \mathbb{R}^n\) and let \(f: \mathbb{R}^n \rightarrow \mathbb{R}\) be a convex function. Then, the composition \(g \overset{\text{def.}}{=} f \circ h\), i.e., \(g(x) = f(Ax + b)\), is again a convex function.

### 1.2 SD-transformation of a submodular function: Problem and Results

This paper is concerned with symmetric difference maps over a 0-1 hypercube, as an analogy of affine maps. Let \(\sigma_S: \{0,1\}^V \rightarrow \{0,1\}^V\) denote a symmetric difference map (SD-map) by a set \(S \subseteq V\), which is given by

\[
\sigma_S(X) \overset{\text{def.}}{=} X \Delta S
\]

for any \(X \subseteq V\), where \(X \Delta S = (X \setminus Y) \cup (Y \setminus X)\) is the symmetric difference between \(X\) and \(S\). For a set function \(f: \{0,1\}^V \rightarrow \mathbb{R}\) and a set \(S \subseteq V\), we say \(g \overset{\text{def.}}{=} f \circ \sigma_S\) is a symmetric difference transformation (SD-transformation) of \(f\) by \(S\), i.e., the SD-transformation is the set function \(g: \{0,1\}^V \rightarrow \mathbb{R}\) given by \(g(X) = f(X \Delta S)\) for any \(X \subseteq V\).

Let \(f\) be a submodular function, and let \(g = f \circ \sigma_S\) be an SD-transformation of \(f\) by \(S\). Notice that \(g\) may not be submodular. However, \(g \circ \sigma_S\) is submodular again, since \(g \circ \sigma_S = f \circ \sigma_S \circ \sigma_S = f\) holds. This paper is concerned with the following problem.

**Problem 1.** Let \(g: \{0,1\}^V \rightarrow \mathbb{R}\) be an SD-transformation of a submodular function. Provided that \(g\) is given by its function value oracle, the goal is to find a subset \(T \subseteq V\) such that \(h = g \circ \sigma_T\) is submodular.

We call a solution \(T\) of Problem 1 canonical set (of an SD-transformation \(g\)). Notice that a canonical set is not unique. In fact, we will show that if \(T\) is a canonical set then \(V \setminus T\) is also a canonical set (see Proposition 3.10 in Section 3.4.2). Figure 1 shows an example. The left figure shows a submodular function \(f: \{0,1\}^{\{1,2,3\}} \rightarrow \mathbb{R}\), and the right figure shows its SD-transformation \(g\) by the set \(\{1,2\}\). Notice that \(g\) is not submodular since \(\Phi_g(\{1\}, \{3\}) = g(\{1\}) + g(\{3\}) - g(\{1,3\}) - g(\emptyset) < 0\). The set \(\{1,2\}\) is a canonical set of \(g\), as well as \(\{3\}, \{1\}\) and \(\{2,3\}\).

Once we find a canonical set \(T\), we can apply many algorithms for submodular functions, such as minimization or maximization, to \(g \circ \sigma_T\). Unfortunately, Problem 1 requires exponentially many oracle calls, in the worst case. An easy example is given as follows (see e.g., [7]). Let \(U \subseteq V\), then we define a set function \(g: \{0,1\}^V \rightarrow \mathbb{R}\) by \(g(U) = -1\) and \(g(X) = 0\) for any other subset \(X \subseteq V\). Then, the canonical sets are only \(U\) and \(V \setminus U\). It is not difficult to observe that Problem 1 requires \(2^{|V|} - 2\) oracle calls in the worst case.
Figure 1: (Left) A submodular function \( f \) on \( V = \{1, 2, 3\} \). (Right) \( g = f \circ \sigma_{\{1, 2\}} \).

### 1.3 Contribution

Concerning Problem 1, this paper presents characterizations of SD-maps preserving the submodularity, i.e., given a submodular function \( f \), we characterize \( S \in \{0, 1\}^V \) for which \( f \circ \sigma_S \) is again submodular. In Section 3, Theorem 3.3 presents a characterization described by a Boolean system. Theorem 3.7 rephrases the characterization in terms of a graph defined for \( f \). By a similar and simpler argument, we can also show that any SD-transformation of modular function is modular (Proposition 3.8).

Then, we present a characterization of the solutions of Problem 1 in Section 4. Theorem 4.1 provides the characterization described by a Boolean system. As an interesting consequence, Theorem 4.2 shows that Problem 1 is solved by calling the function value oracle \( O(|V|) \) times if \( f \) is strictly submodular. Once we find a canonical set of an SD-transformation \( g \) of a submodular function, minimization of \( g \) is easy using submodular function minimization, as we stated above. However, the converse is not true, and Section 4.3 shows that Problem 1 requires function value oracle calls exponential times, even if we have all minimizer (or maximizer) of \( g \).

### 1.4 Related works

**Recognizing submodularity.** Obviously, it takes exponential time to check if a set function given by its function value oracle is submodular, in general. To be precise, the submodularity is confirmed in \( 2^{|V|} \cdot \text{poly}(|V|) \) time, instead of checking \( \Phi_f(X, Y) \geq 0 \) for all \( \binom{2^{|V|}}{2} \simeq (2^{|V|})^2 \) pairs \( X, Y \in \{0, 1\}^{|V|} \) (see Section 2).

Goemans et al. [8] is concerned with approximating a submodular function with polynomially many oracle calls. For nonnegative monotone submodular functions \( f \), they showed that an approximate function \( \tilde{f} \) is constructed by calling \( \text{poly}(|V|) \) times the function value oracle of \( f \), such that \( \tilde{f}(X) \leq f(X) \leq \alpha \tilde{f}(X) \) for any \( X \in \{0, 1\}^{|V|} \) with an approximation factor \( \alpha = O(\sqrt{|V|} / \log |V|) \). Notice that \( \tilde{f} \) may not be submodular. They also gave a lower bound \( \Omega(\sqrt{|V|} / \log |V|) \) of the approximation ratio with polynomially many oracle calls.

**SD-transformation of a submodular function.** Gillenwater et al. [7] are concerned with *submodular Hamming distance* \( d_f(A, B) = f(A \triangle B) \) for \( A, B \subseteq V \) given by a positive polymatroid function \( f \), that is a monotone nondecreasing positive submodular function \( f \) satisfying \( f(\emptyset) = 0 \). Giving some applications in machine learning, such as clustering, structured prediction, and diverse \( k \)-best, they investigated the hardness and approximations of problems SH-min: \( \min_{A \in C} \sum_{i=1}^m f_i(A \triangle B_i) \) and SH-max: \( \max_{A \in C} \sum_{i=1}^m f_i(A \triangle
$B_i$, where $f_i$ is a positive polymatroid, $B_i \subseteq V$, and $C$ denotes a combinatorial constraint.

1.5 Road map

As a preliminary step, Section 2 is concerned with the 2-faces of 0-1 hypercube. More precisely, Section 2.1 mentions the known fact that the submodularity is confirmed only by checking the submodularity on 2-faces. Section 2.2 works up the SD-map $\sigma_S$ on 2-faces.

Section 3 provides characterizations of SD-maps preserving the submodularity. Prior to the main theorems, Section 3.1 proves a key lemma using the argument in Section 2.2. Sections 3.2 and 3.3 respectively show the main theorems. Section 3.4 make some remarks on Section 3.

Then, Section 4 deals with Problem 1. Section 4.1 characterizes canonical sets using a Boolean system. Section 4.2 presents a linear time algorithm of Problem 1 provided that $f$ is strict submodular. Section 4.3 gives some bad examples. Section 5 concludes this paper.

2 Preliminary: 2-faces of a 0-1 hypercube

2.1 Submodularity is determined on 2-faces

Let $X \in \{0, 1\}^V$ and let $u, v \in V$ be a distinct pair. For convenience, let $X' = X \setminus \{u, v\}$ then the four distinct subsets $X', X' \cup \{u\}, X' \cup \{v\}$ and $X' \cup \{u, v\}$ of $V$ form a 2-face (a.k.a. polygonal face) of the $n$-dimensional 0-1 hypercube of the vertex set $\{0, 1\}^V$. Let

$$P \overset{\text{def.}}{=} \left\{ (X, \{u, v\}) \mid X \subseteq V, \{u, v\} \in \binom{V \setminus X}{2} \right\}$$

(3)

denote the whole set of 2-faces of $n$-dimensional hypercube, where $(X, \{u, v\})$ corresponds to the 2-face consisting of $X, X \cup \{u\}, X \cup \{v\}, X \cup \{u, v\}$. Notice that $|P| = 2^{n-2} \binom{n}{2}$ holds (cf., [3]).

For convenience, let $\Phi_f : P \to \mathbb{R}$ be defined by

$$\Phi_f(X, \{u, v\}) \overset{\text{def.}}{=} \Phi_f(X \cup \{u\}, X \cup \{v\})$$

(4)

$$= f(X \cup \{u\}) + f(X \cup \{u\}) - f(X \cup \{u, v\}) - f(X)$$

for any $(X, \{u, v\}) \in P$.

The following characterization of submodular functions is known.

**Theorem 2.1** ([18]). A set function $f : \{0, 1\}^V \to \mathbb{R}$ is submodular if and only if $\Phi_f(p) \geq 0$ holds for any $p \in P$.

2.2 SD-map on 2-faces

In this section, we are concerned with the map over $P$ provided by an SD-map $\sigma_S$ for a subset $S \subseteq V$, as a preliminary step of the arguments in the following sections. It may not be difficult to see that

$$\{\sigma_S(X), \sigma_S(X \cup \{u\}), \sigma_S(X \cup \{v\}), \sigma_S(X \cup \{u, v\})\}$$

again forms a 2-face of a 0-1 hypercube. To be precise, we can show the following proposition.

\[ \text{(For the simplicity of the notation, we use the notation } \Phi(X, \{u, v\}) \text{ instead of } \Phi((X, \{u, v\})). \text{ At the same time, we also use the notation } \Phi(p) \text{ for } p = (X, \{u, v\}) \in P. \]
Proposition 2.2. For each \((X, \{u, v\}) \in \mathcal{P}\),
\[
\{\sigma_S(X), \sigma_S(X \cup \{u\}), \sigma_S(X \cup \{v\}), \sigma_S(X \cup \{u, v\})\} = \{Y, Y \cup \{u\}, Y \cup \{v\}, Y \cup \{u, v\}\}
\]
holds, where \(Y = (X \triangle S) \setminus \{u, v\}\).

Proof. We are concerned with three cases that \(|\{u, v\} \cap S| = 0, 1, \text{ or } 2\).

Case i) Suppose that \(|\{u, v\} \cap S| = 0\), i.e., \(u \not\in S\) and \(v \not\in S\). Notice that \(u \not\in X \triangle S\) and \(v \not\in X \triangle S\).

Thus,
\[
\begin{aligned}
Y & = (X \triangle S) \setminus \{u\} = (X \cup \{u\}) \triangle S \quad (5) \\
Y \cup \{u\} & = (X \triangle S) \cup \{u\} = (X \cup \{u\}) \triangle S \quad (6) \\
Y \cup \{v\} & = ((X \triangle S) \setminus \{u\}) \cup \{v\} = (X \cup \{v\}) \triangle S \quad (7) \\
Y \cup \{u, v\} & = (X \triangle S) \cup \{u, v\} = (X \cup \{u, v\}) \triangle S \quad (8)
\end{aligned}
\]
hold, where the right hind sides are respectively \(\sigma_S(X), \sigma_S(X \cup \{u\}), \sigma_S(X \cup \{v\})\) and \(\sigma_S(X \cup \{u, v\})\).

Then, we obtain the claim in this case.

Case ii) Suppose that \(|\{u, v\} \cap S| = 1\). Without loss of generality, we may assume that \(u \in S\) and \(v \not\in S\). Then,
\[
\begin{aligned}
Y & = (X \triangle S) \setminus \{u\} = (X \cup \{v\}) \triangle S \quad (9) \\
Y \cup \{u\} & = (X \triangle S) \cup \{u\} = (X \triangle S) \quad (10) \\
Y \cup \{v\} & = ((X \triangle S) \setminus \{u\}) \cup \{v\} = (X \cup \{v\}) \triangle S \quad (11) \\
Y \cup \{u, v\} & = (X \triangle S) \cup \{v\} = (X \cup \{v\}) \triangle S \quad (12)
\end{aligned}
\]
hold, where the right hind sides are respectively \(\sigma_S(X \cup \{v\}), \sigma_S(X), \sigma_S(X \cup \{u, v\})\) and \(\sigma_S(X \cup \{u\})\).

Then, we obtain the claim in this case.

Case iii) Suppose that \(|\{u, v\} \cap S| = 2\), i.e., \(u \in S\) and \(v \in S\). Then,
\[
\begin{aligned}
Y & = (X \triangle S) \setminus \{u, v\} = (X \cup \{u, v\}) \triangle S \quad (13) \\
Y \cup \{u\} & = (X \triangle S) \setminus \{u\} = (X \cup \{v\}) \triangle S \quad (14) \\
Y \cup \{v\} & = (X \triangle S) \setminus \{u\} = (X \cup \{u\}) \triangle S \quad (15) \\
Y \cup \{u, v\} & = (X \triangle S) = (X \triangle S) \triangle S \quad (16)
\end{aligned}
\]
hold, where the right hind sides are respectively \(\sigma_S(X \cup \{u, v\}), \sigma_S(X \cup \{v\}), \sigma_S(X \cup \{u\})\) and \(\sigma_S(X)\).

Then, we obtain the claim.

Let \(\tilde{\sigma}_S : \mathcal{P} \to \mathcal{P}\) for \(S \subseteq V\) be defined by
\[
\tilde{\sigma}_S(X, \{u, v\}) \overset{\text{def.}}{=} (Y, \{u, v\}) 
\]
for any \((X, \{u, v\}) \in \mathcal{P}\) where \(Y = (X \triangle S) \setminus \{u, v\}\). Then, \(\tilde{\sigma}_S\) is the map on \(\mathcal{P}\) provided by \(\sigma_S\) by Proposition 2.2. Since \(\sigma_S\) is bijective on \(\{0, 1\}^V\), Proposition 2.2 also implies the following.

Corollary 2.3. \(\tilde{\sigma}_S\) is bijective.

\footnote{For the simplicity of the notation we use \(\tilde{\sigma}_S(X, \{u, v\})\), instead of \(\tilde{\sigma}_S((X, \{u, v\}))\). At the same time, we also use the notation \(\tilde{\sigma}(p)\) for \(p = (X, \{u, v\}) \in \mathcal{P}\).}
3 SD-maps preserving submodularity

This section characterizes $S \subseteq V$ whether $f \circ \sigma_S$ is submodular. Theorem 3.3 describes it using a Boolean system, and Theorem 3.7 rephrases it using a graph. As a preliminary argument, we give a key lemma in Section 3.1

3.1 Key lemma

**Lemma 3.1.** Let $f : \{0, 1\}^V \to \mathbb{R}$ be a submodular function. Suppose that a 2-face $p = (X, \{u, v\}) \in \mathcal{P}$ satisfies that $\widetilde{\Phi}_f(p) > 0$.

Then for any subset $S \subseteq V$,

$$\widetilde{\Phi}_{f \circ \sigma_S}(\tilde{\sigma}_S(p)) > 0$$  (18)

holds if and only if $|S \cap \{u, v\}| \equiv 0 \pmod{2}$.

**Proof.** By Proposition 2.2 and the definition (4) of $\widetilde{\Phi}_f$, the condition (18) holds if and only if $f \circ \sigma_S(Y \cup \{u\}) + f \circ \sigma_S(Y \cup \{v\}) > f \circ \sigma_S(Y \cup \{u, v\}) + f \circ \sigma_S(Y)$

holds on the 2-face $(Y, \{u, v\}) = \tilde{\sigma}(X, \{u, v\})$, where $Y = (X \symdiff S) \setminus \{u, v\}$.

$(\Leftarrow)$ We show that (18) holds if $|\{u, v\} \cap S| = 0$ or 2. If $|\{u, v\} \cap S| = 0$, then

$$\widetilde{\Phi}_{f \circ \sigma_S}(\tilde{\sigma}_S(X, \{u, v\}))$$

$$= f \circ \sigma_S(Y \cup \{u\}) + f \circ \sigma_S(Y \cup \{v\}) - (f \circ \sigma_S(Y \cup \{u, v\}) + f \circ \sigma_S(Y))$$

$$= f((Y \cup \{u\}) \symdiff S) + f((Y \cup \{v\}) \symdiff S) - (f((Y \cup \{u, v\}) \symdiff S) + f(Y \symdiff S))$$

$$= f(X \cup \{u\}) + f(X \cup \{v\}) - (f(X \cup \{u, v\}) + f(X))$$

(by (5)–(8))

$$= \tilde{\Phi}_f(X, \{u, v\})$$

$$> 0$$

hold, where the last inequality follows the hypothesis that $\tilde{\Phi}_f(p) > 0$.

If $|\{u, v\} \cap S| = 2$, i.e., $u \in S$ and $v \in S$, then

$$\widetilde{\Phi}_{f \circ \sigma_S}(\tilde{\sigma}_S(X, \{u, v\}))$$

$$= f \circ \sigma_S(Y \cup \{u\}) + f \circ \sigma_S(Y \cup \{v\}) - (f \circ \sigma_S(Y \cup \{u, v\}) + f \circ \sigma_S(Y))$$

$$= f((Y \cup \{u\}) \symdiff S) + f((Y \cup \{v\}) \symdiff S) - (f((Y \cup \{u, v\}) \symdiff S) + f(Y \symdiff S))$$

$$= f(X \cup \{v\}) + f(X \cup \{u\}) - (f(X) + f(X \cup \{u, v\}))$$

(by (13)–(16))

$$= \tilde{\Phi}_f(X, \{u, v\})$$

$$> 0$$

hold, where the last inequality follows the hypothesis that $\tilde{\Phi}_f(p) > 0$. We obtain the claim.
We prove the contraposition: if $|S \cap \{u, v\}| = 1$ then (18) does not hold. Without loss of generality we may assume that $u \in S$ and $v \not\in S$. Then

\[
\begin{align*}
\tilde{\Phi}_{f \circ \sigma_S}(\hat{\sigma}_S(X, \{u, v\})) &= f \circ \sigma_S(Y \cup \{u\}) + f \circ \sigma_S(Y \cup \{v\}) - (f \circ \sigma_S(Y \cup \{u, v\}) + f \circ \sigma_S(Y)) \\
&= f(Y \cup \{u\}) \Delta S + f((Y \cup \{v\}) \Delta S) - (f((Y \cup \{u, v\}) \Delta S) + f(Y \Delta S)) \\
&= f(X) + f(X \cup \{u, v\}) - f(X \cup \{u\}) + f(X \cup \{v\}) \quad \text{(by (9)--(12))} \\
&= -\tilde{\Phi}_f(X, \{u, v\}) \\
< 0
\end{align*}
\]

hold, where the last inequality follows the hypothesis that $\tilde{\Phi}_f(p) > 0$. Now, we obtain the claim. □

The proof for the following lemma is similar to and much easier than the one for Lemma 3.2, so that we omit it.

**Lemma 3.2.** Let $f : \{0, 1\}^V \to \mathbb{R}$ be a submodular function. Suppose that a 2-face $p \in \mathcal{P}$ satisfies that $\tilde{\Phi}_f(p) = 0$. Then for any subset $S \subseteq V$,

\[
\tilde{\Phi}_{f \circ \sigma_S}(\hat{\sigma}_S(p)) = 0
\]

holds. □

### 3.2 A characterization by a Boolean system

This section presents a characterization of SD-maps which preserve submodularity, as a consequence of Lemmas 3.1 and 3.2. For any set function $f : \{0, 1\}^V \to \mathbb{R}$, we define a matrix $M_f \in \{0, 1\}^{\mathcal{P} \times V}$ where, its $(X, \{u, v\})$-th row vector is given by

\[
M_f[(X, \{u, v\}), \cdot] = \begin{cases} 
\chi_S^\top \{u, v\} & \text{if } \tilde{\Phi}_f(X, \{u, v\}) \neq 0, \\
0^\top & \text{otherwise},
\end{cases}
\]

(19)

for each $(X, \{u, v\}) \in \mathcal{P}$, where $\chi_S \in \{0, 1\}^V$ denotes the characteristic (column) vector of $S \subseteq V$, i.e., $\chi_S(w) = 1$ if $w \in S$; otherwise $\chi_S(w) = 0$. Then an SD-map $\sigma_S$ that preserves the submodularity of a submodular function $f$ is characterized by the next theorem.

**Theorem 3.3.** Let $f : \{0, 1\}^V \to \mathbb{R}$ be a submodular function. For any $S \subseteq V$, $f \circ \sigma_S$ is submodular if and only if $M_f \chi_S \equiv 0 \pmod{2}$ holds.

We need the following lemma to show Theorem 3.3.

**Lemma 3.4.** Let $f : \{0, 1\}^V \to \mathbb{R}$ be a submodular function. For any $S \subseteq V$ and for any $p = (X, \{u, v\}) \in \mathcal{P}$, $\tilde{\Phi}_{f \circ \sigma_S}(\hat{\sigma}_S(p)) \geq 0$ if and only if

\[
M_f[p, \cdot] \chi_S \equiv 0 \pmod{2}
\]

holds.
Proof. The proof is by a case analysis of \((X, \{u,v\}) \in P\). If \(\tilde{\Phi}_f(X, \{u,v\}) = 0\) holds for \((X, \{u,v\}) \in P\), then \(M_f[(X, \{u,v\}), \cdot] = 0\) holds by the definition of \(M_f\). Using Lemma 3.2, the claim is easy in this case. Suppose that \(\tilde{\Phi}_f(X, \{u,v\}) \neq 0\) holds for \((X, \{u,v\}) \in P\). Then,

\[M_f[(X, \{u,v\}), \cdot] \chi_S = \chi_S(u) + \chi_S(v) = |\{u,v\} \cap S|\]

by the definition of \(M_f\). Now the claim follows from Lemma 3.1.

Proof of Theorem 3.3. Since \(\tilde{\sigma}_S\) is bijective on \(P\) by Corollary 2.3, \(\tilde{\Phi}_f \circ \sigma_S(\tilde{\sigma}_S(p)) \geq 0\) holds for any \(p \in P\) implies that \(\tilde{\Phi}_f(\sigma_S(p)) \geq 0\) holds for any \(p \in P\). Now, Theorem 3.3 is immediate from Lemma 3.4, using Theorem 2.1.

3.3 An interpretation of Theorem 3.3 by a graph

Section 3.3 shows Theorem 3.7, which is regarded as an interpretation of Theorem 3.3 in terms of a graph.

To begin with, the Boolean system \(M_f \chi_S \equiv 0 \pmod{2}\) considered in Theorem 3.3 contains many redundant constraints since the rank of the matrix \(M_f \in \{0, 1\}^{P \times V}\) is at most \(|V|\). Then, we define the reduced matrix \(\overline{M}_f \in \{0, 1\}^{V/2 \times V}\) of \(M_f\) where its \(\{u,v\}\)-th row vector (\(\{u,v\} \in \binom{V}{2}\)) is given by

\[
\overline{M}_f[\{u,v\}, \cdot] = \begin{cases} 
\chi_{\{u,v\}}^T & \text{if there is an } (X, \{u,v\}) \in P \text{ such that } \tilde{\Phi}_f(X, \{u,v\}) \neq 0, \\
0 & \text{otherwise},
\end{cases}
\]

for each \(\{u,v\} \in \binom{V}{2}\). Now we make an observation, whose proof is (almost) trivial, so that we omit it.

Observation 3.5. For any \(\chi \in \{0, 1\}^V\), \(M_f \chi \equiv 0 \pmod{2}\) if and only if \(\overline{M}_f \chi \equiv 0 \pmod{2}\).

We can regard \(\overline{M}_f\) as the (redundant) incidence matrix of what is called the inequality graph \(G_f\) of \(f\). Precisely, for any set function \(f: \{0, 1\}^V \to \mathbb{R}\), let \(G_f = (V, E_f)\) be an undirected graph with the edge set

\[
E_f \overset{\text{def}}{=} \left\{ \{u,v\} \in \binom{V}{2} \mid \exists (X, \{u,v\}) \in P, \tilde{\Phi}_f(X, \{u,v\}) \neq 0 \right\}.
\]

Figure 2 shows the inequality graph of the submodular function \(f\) given in Figure 1.

The following observation is also trivial (see also the arguments on the graphic matroid [5]).

Observation 3.6. For any \(S \subseteq V\), \(\overline{M}_f \chi_S \equiv 0 \pmod{2}\) holds if and only if \(\chi_S(u) = \chi_S(v)\) holds for any \(\{u,v\} \in E_f\).

---

\[\text{This reduction itself does not reduce the time complexity: to construct } \overline{M}_f \text{ we have to check (almost) all } (X, \{u,v\}) \in P \text{ in the worst case, to confirm if } \exists X \subseteq V \setminus \{u, v\} \text{ satisfying the condition. See Proposition 4.3.}\]

8
Observation 3.6 implies that $S$ is a canonical set if and only if every connected component of $G_f$ is included in or completely excluded from $S$. To be precise, let $U_i \subseteq V$ ($i = 1, \ldots, k$) be the connected components of $G_f$ where $k$ is the number of connected components of $G_f$. Let $\mathcal{U}(f)$ denote the whole set family of unions of $U_i$ ($i = 1, \ldots, k$), i.e.,

$$\mathcal{U}(f) = \left\{ \bigcup_{i \in I} U_i \mid I \subseteq \{1, 2, \ldots, k\} \right\}. \quad (22)$$

Now we can conclude the following theorem as an easy consequence of Theorem 3.3 and Observations 3.5 and 3.6.

**Theorem 3.7.** For any submodular function $f : \{0, 1\}^V \to \mathbb{R}$, $f \circ \sigma_S$ is submodular if and only if $S \in \mathcal{U}(f)$.

### 3.4 Remarks of Section 3

This section makes some remarks concerning the arguments in Section 3. Sections 3.4.1 and 3.4.2 are easy implications of Lemmas 3.1 and 3.2. Sections 3.4.3, 3.4.4 and 3.4.5 are remarks on Theorem 3.7.

#### 3.4.1 SD-transformation of a modular function

**Proposition 3.8.** If a set function $f : \{0, 1\}^V \to \mathbb{R}$ is modular then $f \circ \sigma_S$ is modular for any $S \subseteq V$.

**Proof.** The claim is immediate from Lemma 3.2. We will use Proposition 3.8 in Section 4.3.

#### 3.4.2 Complement of a canonical set

**Proposition 3.9.** If a set function $f : \{0, 1\}^V \to \mathbb{R}$ is submodular then $f \circ \sigma_V$ is submodular.

**Proof.** Notice that $M_f \chi_V = 0$ holds by the definition (19) of $M_f$. The claim is immediate from Theorem 3.3.

The following proposition is a corollary of Proposition 3.9.

**Proposition 3.10.** Let $g : \{0, 1\}^V \to \mathbb{R}$ be an SD-transformation of a submodular function. If $T \subseteq V$ is a canonical set of $g$, so is $V \setminus T$.

**Proof.** By the hypothesis, $h = g \circ \sigma_T$ is submodular. Proposition 3.9 implies that $h' = h \circ \sigma_V$ is submodular. Since the symmetric difference is commutative and associative, we see that $h' = h \circ \sigma_V = g \circ \sigma_T \circ \sigma_V = g \circ \sigma_V \setminus S$, and we obtain the claim.

#### 3.4.3 Nontrivial example of many canonical sets

Using Theorem 3.7, we give a nontrivial example of submodular functions which have many canonical sets. For any finite set $V$ and any partition $U_1, U_2, \ldots, U_k$ of $V$, let $f : \{0, 1\}^V \to \mathbb{R}$ be a set function defined by

$$f(X) = \min_{W \in \mathcal{U}} |X \Delta W| \quad (23)$$

for any $X \subseteq V$, where $\mathcal{U} = \left\{ \bigcup_{i \in I} U_i \mid I \subseteq \{1, 2, \ldots, k\} \right\}$.

This function represents the edit distance from the nearest point in the Boolean sublattice $\mathcal{U}$ of $\{0, 1\}^V$. 

9
Figure 3: (Left) Submodular function $f$ given by (24) on $V = \{1, 2, 3\}$. (Right) The inequality graph $G_f$.

**Proposition 3.11.** The set function $f$ given by (23) is submodular.

**Proposition 3.12.** For the submodular function $f$ given by (23), $f \circ \sigma_S$ is submodular if and only if $S \in U$.

See Appendix A for the proofs of Propositions 3.11 and 3.12.

### 3.4.4 A connected component of an inequality graph is not a clique, in general

As for the inequality graph of a submodular function defined by (21), it would be natural to ask if $U_i$ is a clique, considering the transitivity of $=$. However, it is not the case. Let $V = \{1, 2, 3\}$, and let $f: \{0, 1\}^V \to \mathbb{R}$ be a set function given by

$$f(X) = \begin{cases} 0 & \text{if } X = \emptyset, \\ 2 & \text{if } X = \{1, 3\}, \\ 1 & \text{otherwise}, \end{cases}$$  \hspace{1cm} (24)

for $X \in \{0, 1\}^V$ (see Figure 3 left). We can check that $f$ is submodular by Theorem 2.1. Then, its inequality graph is given by $G_f = (V, \{(1, 2), (2, 3)\})$, since $\Phi_f(\emptyset, \{1, 3\}) = \Phi_f(\{2\}, \{1, 3\}) = 0$, $\Phi_f(\emptyset, \{x, y\}) = 1 \neq 0$, $\Phi_f(\emptyset, \{y, z\}) = 1 \neq 0$ (see Figure 3 right). Clearly, the unique connected component of $G_f$ is not a clique.

### 3.4.5 Connection to the inseparable decomposition

For a submodular function $f: \{0, 1\}^V \to \mathbb{R}$, a nonempty set $U \subseteq V$ is **separable** if there exists $X \subset U$ ($U \neq \emptyset$) such that $\Phi_f(U, U \setminus X) = 0$ holds. Otherwise $U$ is **inseparable**[2, 16, 11, 5, 6].

**Theorem 3.13** (see e.g., [11, 6]). For a submodular function $f: \{0, 1\}^V \to \mathbb{R}$, $V$ is uniquely partitioned into inseparable subsets $U_1, \ldots, U_k$ with an appropriate $k$. For this partition,

$$f(X) - f(\emptyset) = \sum_{i=1}^k (f(X \cap U_i) - f(\emptyset))$$  \hspace{1cm} (25)

5 Let $\rho(X) = f(X) - f(\emptyset)$ for $X \in \{0, 1\}^V$, then $\rho$ is submodular and $\rho(\emptyset) = 0$. A subset $U$ is separable if $\rho(U) = \rho(X) + \rho(U \setminus X)$[11, 5, 6].
for any $X \in \{0, 1\}^V$. Moreover, this partition is constructible in polynomial time.\footnote{That is $\rho(X) = \sum_{i=1}^k \rho(X \cap U_i)$.}

In fact, the inseparable decomposition of a submodular function is closely related to or essentially the same as the connected components of the inequality graph. More precisely, we can show that $U_1, \ldots, U_k$ are inseparable decomposition of $f$ if and only if each $U_i$ is a vertex set of a connected component of the inequality graph $G_f$. See Appendix B for more details. Thus, the following theorem is an easy consequence of Theorems 3.7 and 3.13.

**Theorem 3.14.** Given a submodular function $f : \{0, 1\}^V \to \mathbb{R}$ by its function value oracle, and given $S \subseteq V$, the question if $f \circ \sigma_S$ is submodular is decided in polynomial time.

**Proof.** The inseparable decomposition of $f$ is found in polynomial time by Theorem 3.13, where the decomposition $U_1, \ldots, U_k$ corresponds to the connected components of the inequality graph $G_f$ (see Proposition B.1). By Theorem 3.7, $f \circ \sigma_S$ is submodular if and only if $S \in U(f)$. The latter condition is checkable in linear time.

We emphasize that Theorem 3.14 does not imply Problem 1 is solved in polynomial time, at all. The next section is concerned with Problem 1, using the characterizations given in this section.

### 4 Finding A Canonical Set

#### 4.1 A characterization of canonical sets

Now, we go back to Problem 1. For any set function $g : \{0, 1\}^V \to \mathbb{R}$, let $b_g \in \{0, 1\}^\mathcal{P}$ be defined by

$$b_g[(Z, \{u, v\})] = \begin{cases} 0 & \text{if } \hat{\Phi}_g(Z, \{u, v\}) \geq 0, \\ 1 & \text{otherwise}, \end{cases}$$

for any $(Z, \{u, v\}) \in \mathcal{P}$.\footnote{It takes $O(n^2)$ time if we have a base of $f$ (see \cite{6,5}).}

**Theorem 4.1.** Let $g : \{0, 1\}^V \to \mathbb{R}$ be an SD-transformation of a submodular function. Then, $h = g \circ \sigma_T$ for $T \subseteq V$ is submodular if and only if

$$M_g \chi_T \equiv b_g \pmod{2}$$

holds where $\chi_T$ is the characteristic vector of $T$.

**Proof.** Suppose that $g$ is given by $g = f \circ \sigma_S$ for a submodular function $f$ and $S \subseteq V$. Firstly, we claim that

$$M_g \chi_S \equiv b_g \pmod{2}$$

holds. By Lemma 3.4, $\hat{\Phi}_g(\sigma_S(X, \{u, v\})) \geq 0$ if and only if $M_f[(X, \{u, v\}), \cdot] \chi_S \equiv 0 \pmod{2}$. By the definition (19) of $M_f$, and Lemmas 3.1 and 3.2,

$$M_g[\sigma_S(X, \{u, v\}), \cdot] = M_f[(X, \{u, v\}), \cdot]$$

holds for any $(X, \{u, v\}) \in \mathcal{P}$. Thus, $\hat{\Phi}_g(\sigma_S(X, \{u, v\})) \geq 0$ if and only if $M_g[\sigma_S(X, \{u, v\}), \cdot] \chi_S \equiv 0 \pmod{2}$. This implies (27), since $\sigma_S$ is bijective on $\mathcal{P}$ by Corollary 2.3.
Then, (27) and the hypothesis that $M_g \chi_T = b_g$ imply that
\[ M_g \chi_S + M_g \chi_T \equiv b_g + b_g \equiv 0 \pmod{2} \] (29)
holds. Meanwhile,
\[ M_g \chi_T + M_g \chi_S = M_g (\chi_T + \chi_S) \] (30)
holds. Notice that $\chi_S \triangle T \equiv \chi_S + \chi_T \pmod{2}$ holds. Thus, (29) and (30) imply that
\[ M_g \chi_S \triangle T \equiv 0 \pmod{2} \] (31)
holds. By (28), (31) also implies
\[ M_f \chi_S \triangle T \equiv 0 \pmod{2} \] (32)
holds. Then, $f \circ \sigma_{S \triangle T}$ is submodular by Theorem 3.3. It is easy to observe that
\[ g \circ \sigma_T = f \circ \sigma_S \circ \sigma_T = f \circ \sigma_{S \triangle T} \]
holds, and we obtain the claim. \qed

4.2 Linear-time algorithm for strictly submodular function

What is interesting is that Problem 1 is solvable in linear time for strictly submodular function. Precisely, it is described as follows.

**Theorem 4.2.** Problem 1 is solved in $2|V| \cdot EO + O(|V|)$ time if the set function $f$ is strictly submodular, where $EO$ denotes the time complexity of an oracle call to know the value of $g(X)$ for a set $X \subseteq V$.

**Proof.** Since $f$ is strictly submodular, $G_f$ is connected. In particular, let $u^* \in V$ be arbitrary. Then $\Phi_g(\emptyset, \{u^*, v\}) \neq 0$ holds for any $v \in V \setminus \{u^*\}$. Thus, we can obtain a canonical set $T \subseteq V$ by solving the Boolean system $M_g[(\emptyset, \{u^*, v\}), \chi_T] \equiv b_g[(\emptyset, \{u^*, v\})] \pmod{2}$ for $v \in V \setminus \{u^*\}$. (Recall (19) and (26) for the definitions of $M_g$ and $b_g$.)

In fact, the solution of the Boolean system is simply given as follows: Set $T := \emptyset$ for initialization. For each $v \in V \setminus \{u^*\}$, set $T := T \cup \{v\}$ if $\Phi_g(\emptyset, \{u^*, v\}) < 0$. See Algorithm 1 for a formal description. It is not difficult to observe that the obtained $T$ provides a solution of the Boolean system by Observation 3.6. Computing $\Phi_g(\emptyset, \{u^*, v\})$ requires the values of $g(\emptyset)$, $g(\{u^*\})$, $g(\{v\})$ and $g(\{u^*, v\})$ for $v \in V \setminus \{u^*\}$.

Now the time complexity is easy. \qed

**Algorithm 1.**

Given a function value oracle of $g$: \{0, 1\}^V \rightarrow \mathbb{R}$.
Set $T := \emptyset$. Choose $u^* \in V$ arbitrarily.
Get the values $g(\emptyset)$ and $g(\{u^*\})$.
For each $v \in V \setminus \{u^*\}$,
Get the values $g(\{v\})$ and $g(\{u^*, v\})$.
If $\Phi_g(\emptyset, \{u^*, v\}) < 0$, then set $T := T \cup \{v\}$.
Output $T$. 12
4.3 Minimizer/Maximize is helpless for finding a canonical set

Once we obtain a canonical set \( T \) for an SD-transformation \( g \) of a submodular function, we can find the minimum value of \( g \) using a submodular function minimization algorithm. However the opposite is not always true; finding a canonical set is sometimes hard even if all minimizers of \( g \) are given.

**Proposition 4.3.** Problem \( 1 \) requires \( 2^{|V|} - 2 \) function value oracle calls in the worst case, even if all minimizer of \( g \) are given.

**Proof.** We give an instance of Problem \( 1 \) with a unique minimizer, for which any algorithm needs to call the function value oracle at least \( 2^{|V|} - 2 \) times to solve Problem \( 1 \). For any \( U \subseteq V \) such that \( U \neq \emptyset \), let \( g_U : \{0, 1\}^V \rightarrow \mathbb{R} \) be a set function defined by

\[
g_U(X) = \begin{cases} |X| - \frac{1}{2} & \text{(if } X = U), \\ |X| & \text{(otherwise),} \\ \end{cases}
\]

for \( X \in \{0, 1\}^V \). Observe that \( g_U(X) > 0 \) for any \( X \neq \emptyset \), meaning that \( \emptyset \) is the unique minimizer of \( g_U \) with the minimum value \( g_U(\emptyset) = 0 \). We claim that exactly \( U \) and \( V \setminus U \) are the canonical sets of \( g_U \). Let

\[
r_U(X) = \begin{cases} -\frac{1}{2} & \text{(if } X = U), \\ 0 & \text{(otherwise) } \end{cases}
\]

for \( X \in \{0, 1\}^V \), and let \( d(X) \overset{\text{def}}{=} |X| \) for \( X \in \{0, 1\}^V \). Then,

\[
g_U(X) = r_U(X) + d(X)
\]

holds. Clearly \( r_U \circ \sigma_U \) is submodular. Since \( d \) is a modular function, \( d \circ \sigma_U \) is again modular by Proposition \( 3.8 \). Notice that

\[
g_U \circ \sigma_U = (r_U + d) \circ \sigma_U = r_U \circ \sigma_U + d \circ \sigma_U
\]

holds. Since the sum of submodular functions is submodular \( 5 \), \( g_U \circ \sigma_U \) is submodular, meaning that \( U \) is a canonical set of \( g \). It is easy to observe \( G_{r_U} \) is connected, and hence \( G_{g_U} = G_f \) is connected since \( d \) is modular. By Theorem \( 3.7 \), we see that only \( U \) and \( V \setminus U \) are canonical sets of \( g \).

To prove that no algorithm finds a canonical set of \( g_U \) with \( 2^{|V|} - 3 \) function value oracle calls, we show the existence of an adversarial oracle. Suppose that an arbitrary algorithm calls the value oracle of \( g_U \) \( 2^{|V|} - 3 \) times. For the \( 2^{|V|} - 3 \) queries, our adversarial oracle answers their cardinalities. Let \( X, Y, Z \in \{0, 1\}^V \) be the remaining sets. Without loss of generality, we may assume that both \( X \neq V \setminus Y \) and \( X \neq V \setminus Z \) hold. (Remark that \( Z = V \setminus Y \) may hold.) Since only \( U \) and \( V \setminus U \) are the canonical sets of \( g_U \), both \( X \) and \( Y \) cannot be canonical sets at the same time. This implies that the algorithm cannot determine \( X, Y \) or \( Z \); if the algorithm answers \( X \) then our oracle can set \( Y = U \), meaning that \( X \) is a wrong answer, and if the algorithm answers \( Y \) or \( Z \) then our oracle can set \( X = U \).

In contrast to minimization, maximization of a submodular function, e.g., max cut, is NP-hard. Even if all maximizers are given, finding a canonical set is hard. The SD-transformation \( g_U \) given in the proof of Proposition \( 4.3 \) also witnesses it.

**Corollary 4.4.** Problem \( 1 \) requires \( 2^{|V|} - 2 \) function value oracle calls in the worst case, even if all maximizer of \( g \) are given.

**Proof.** Let \( U \subseteq V \) satisfy \( U \neq V \) and let \( g_U \) be a set function defined by \( 33 \). Clearly, \( V \) is the unique maximizer of \( g \) with the maximum value \( g(V) = |V| \). Finding canonical set of \( g \) requires \( 2^{|V|} - 2 \) oracle calls, by the same argument as Proposition \( 4.3 \). \( \square \)
5 Concluding Remark

This paper has been concerned with SD-transformations of submodular functions. We gave characterizations of SD-transformations preserving the submodularity in Section 3. We also showed that canonical sets are found in linear time for SD-transformations of a strictly submodular functions in Section 4. It is a natural question if there is another interesting class of submodular functions for which a canonical set is found efficiently. A related question is if there is a nontrivial class of transformations (maps) preserving the submodularity.

We remark that it is not difficult to extend the results to submodular functions on distributive lattices, instead of Boolean lattices. Extensions to submodular functions on a general lattice, i.e., containing $M_3$ or $N_5$, $L$-convex functions and $M$-convex functions \cite{14} on integer lattice, or $k$-submodular functions are interesting.

Acknowledgments

The authors would like to thank Naoyuki Kamiyama for the note on the inseparable decomposition. The authors are also grateful to Satoru Fujishige and Yusuke Kobayashi for their valuable comments. This work is partly supported by JST PRESTO Grant Number JPMJPR16E4, Japan.

References

[1] F. Bach, Learning with Submodular Functions: A Convex Optimization Perspective, Foundations and Trends in Machine Learning, 6:2–3, (2013) 145–373.

[2] R. E. Bixby, W. H. Cunningham and D. M. Topkis, The partial order of a polymatroid extreme point, Mathematics of Operations Research, 10:3 (1985), 367–378.

[3] H. S. M. Coxeter, Regular Polytopes, Dover, 1973.

[4] U. Feige, V. Mirrokni and J. Vondrák, Maximizing non-monotone submodular functions, Proc. the 48th Annual IEEE Symposium on Foundations of Computer Science (FOCS 2007), 461–471.

[5] S. Fujishige, Submodular Functions and Optimization, Second Edition, Elsevier, 2005.

[6] S. Fujishige, A note on submodular function minimization by Chubanov’s LP algorithm, Optimization online, 6217, 2017.

[7] J. A. Gillenwater, R. K. Iyer, B. Lusch, R. Kidambi and J. A. Bilmes, Submodular Hamming metrics, Proc. the 28th International Conference on Neural Information Processing Systems (NIPS 2015), 3141–3149.

[8] M. X. Goemans, N. J. A. Harvey, S. Iwata and V. S. Mirrokni, Approximating submodular functions everywhere, Proc. the 20th Annual ACM-SIAM Symposium on Discrete Algorithms (SODA 2009), 535–544.

[9] S. Iwata, L. Fleischer and S. Fujishige, A combinatorial, strongly polynomial-time algorithm for minimizing submodular functions, Journal of the ACM, 48 (2001), 761–777.

[10] S. Iwata and J. Orlin, A simple combinatorial algorithm for submodular function minimization, Proc. the 20th Annual ACM-SIAM Symposium on Discrete Algorithms (SODA 2009), 1230–1237.
A Supplemental Proofs in Section 3.4.3

This section proves Propositions 3.11 and 3.12. The set function which we are concerned with here is given by

\[ f(X) = \min_{W \in \mathcal{U}} |X \triangle W| \quad \text{(recall (23))} \]

for \( X \in \{0, 1\}^V \), where \( \mathcal{U} = \bigcup_{I \subseteq \{1, 2, \ldots, k\}} U_I \) for a partition \( U_1, \ldots, U_k \) of \( V \).

A.1 Proof of Proposition 3.11

**Proposition A.1** (Proposition 3.11). The set function \( f \) given by (23) is submodular.

**Proof.** Since \( U_1, \ldots, U_k \) is a partition of \( V \), we remark that

\[
|X \triangle W| = \sum_{i=1}^{m} |(X \triangle W) \cap U_i| \\
= \sum_{i=1}^{m} |(X \cap U_i) \triangle (W \cap U_i)|
\]

holds for any \( X \in \{0, 1\}^V \) and \( W \in \mathcal{U} \). Notice that

\[
|(X \cap U_i) \triangle (W \cap U_i)| = \begin{cases} 
|U_i \setminus X| & \text{if } U_i \subseteq W, \\
|X \cap U_i| & \text{otherwise, i.e., } U_i \cap W = \emptyset \text{ since } W \in \mathcal{U},
\end{cases}
\]

(36)
holds for any $X \in \{0, 1\}^V$. For convenience, we define $h_U : \{0, 1\}^V \to \mathbb{R}$ for $U \subseteq V$ by

$$h_U(X) \overset{\text{def.}}{=} \min\{|X \cap U|, |U \setminus X|\} \quad (37)$$

for $X \in \{0, 1\}^V$. Then, $f(X) = \sum_{i=1}^m h_U_i(X)$ holds for any $X \in \{0, 1\}^V$. We will prove that $h_U(X)$ is submodular in the following Lemma A.2. Since the sum of submodular functions is again submodular (see e.g., [5]), we obtain the claim.

**Lemma A.2.** The set function $h_U$ defined by (37) is submodular.

**Proof.** For convenience, let $X' = X \cap U$ and $Y' = Y \cap U$, where we may assume that $|X'| = |X \cap U| \leq |Y'| = |Y \cap U|$ holds, without loss of generality. Notice that

$$h_U(X) = \begin{cases} |X \cap U| = |X'| & \text{if } |X'| \leq |U|/2, \\ |U \setminus X| = |U \setminus X'| = |U| - |X'| & \text{otherwise}, \end{cases} \quad (38)$$

holds for any $X \in \{0, 1\}^V$. We consider the following three cases.

Case i) Suppose that $|X'| \leq |U|/2$ and $|Y'| \leq |U|/2$ hold. Then, $h_U(X) = |X'|$ and $h_U(Y) = |Y'|$ hold. Since $|X' \cap Y'| \leq |X'| \leq |U|/2$,

$$h_U(X \cap Y) = \min\{|(X \cap Y) \cap U|, |U \setminus (X \cap Y)|\} = |X' \cap Y'|$$

holds. Notice that

$$h_U(X \cup Y) = \min\{|(X \cup Y) \cap U|, |U \setminus (X \cup Y)|\} \leq |(X \cup Y) \cap U| = |X' \cup Y'|$$

always holds. Thus,

$$\Phi_{h_U}(X, Y) = h_U(X) + h_U(Y) - h_U(X \cup Y) - h_U(X \cap Y) \geq |X'| + |Y'| - |X' \cup Y'| - |X' \cap Y'| = 0$$

holds where the last equality follows that the cardinality function is modular. We obtain the claim in the case.

Case ii) Suppose that $|X'| > |S|/2$ and $|Y'| > |S|/2$ hold. Then, $h_U(X) = |U| - |X'|$ and $h_U(Y) = |U| - |Y'|$ hold. Since $|X' \cup Y'| \geq |Y'| > |U|/2$,

$$h_U(X \cup Y) = \min\{|(X \cup Y) \cap U|, |U \setminus (X \cup Y)|\} = |U \setminus (X \cup Y)| = |U| - |X' \cup Y'|$$

holds. Notice that

$$h_U(X \cap Y) = \min\{|(X \cap Y) \cap U|, |U \setminus (X \cap Y)|\} \leq |U \setminus (X \cap Y)| = |U| - |X' \cap Y'|$$

always holds. Thus,

$$\Phi_{h_U}(X, Y) = h_U(X) + h_U(Y) - h_U(X \cup Y) - h_U(X \cap Y) \geq |U| - |X' \cup Y'| - |X' \cap Y'| = 0$$

holds where the last equality follows that the cardinality function is modular. We obtain the claim in the case.
always holds. Thus,
\[
\Phi_{h_U}(X, Y) = h_U(X) + h_U(Y) - h_U(X \cup Y) - h_U(X \cap Y) \\
\geq (|U| - |X'|) + (|U| - |Y'|) - (|U| - |X' \cup Y'|) - (|U| - |X' \cap Y'|) = 0
\]
holds where the last equality follows that the cardinality function is modular. We obtain the claim in the case.

Case iii) Suppose that \(|X'| \leq |S|/2\) and \(|Y'| > |S|/2\) hold. Then, \(h_U(X) = |X'|\) and \(h_U(Y) = |U| - |Y'|\) hold. Since \(|X' \cup Y'| \geq |Y'| > |U|/2\),
\[
h_U(X \cup Y) = \min\{|(X \cup Y) \cap U|, |U \setminus (X \cup Y)|\} = |U| - |X' \cup Y'|
\]
holds. Similarly, since \(|X' \cap Y'| \leq |Y'| \leq |U|/2\),
\[
h_U(X \cap Y) = \min\{|(X \cap Y) \cap U|, |U \setminus (X \cap Y)|\} = |X' \cap Y'|
\]
holds. Thus,
\[
\Phi_{h_U}(X, Y) = h_U(X) + h_U(Y) - h_U(X \cup Y) - h_U(X \cap Y) \\
= |X'| + (|U| - |Y'|) - (|U| - |X' \cup Y'|) - (|X' \cap Y'|) \\
= 2|U| + (|X'| - |X' \cup Y'|) + (|X' \cup Y'| - |Y'|) \\
\geq 0
\]
holds. We obtain the claim. \(\square\)

A.2 Proof of Proposition 3.12

**Proposition A.3** (Proposition [3.12]). For the submodular function \(f\) given by (23), \(f \circ \sigma_S\) is submodular if and only if \(S \in \mathcal{U}\).

**Proof.** (\(\Leftarrow\)) We show that \(S \in \mathcal{U}\) is a canonical set. Let \(g = f \circ \sigma_S\), then
\[
g(X) = f \circ \sigma_S(X) = f(X \triangle S) = \min_{W \in \mathcal{U}} |(X \triangle S) \triangle W| = \min_{W \in \mathcal{U}} |X \triangle (S \triangle W)|
\]
(39)
holds for any \(X \in \{0, 1\}^V\). Notice that \(W' = W \triangle S\) is in \(\mathcal{U}\) for any \(W \in \mathcal{U}\) and \(S \in \mathcal{U}\). Thus,
\[
\text{(39)} = \min_{W' \in \mathcal{U}} |X \triangle W'|
\]
holds, which implies that \(g = f\) in fact, and hence \(g\) is submodular (by Proposition [3.11]).

(\(\Rightarrow\)) We prove the contraposition: if \(S \notin \mathcal{U}\) then \(g = f \circ \sigma_S\) is not submodular. By the hypothesis that \(S \notin \mathcal{U}\), there exists \(U_i\) such that \(S \cap U_i \neq \emptyset\) and \(S \cap U_i \neq U_i\). Let \(X = S \Delta U_i\), and we claim that \(\Phi_g(X, S) < 0\). Remark that \(g(X) = g(U_i \triangle S) = f(U_i) = 0\) and \(g(S) = f(\emptyset) = 0\) hold. Then,
\[
g(X \cup S) = g(S \cup U_i) = f((S \cup U_i) \triangle S) = f(U_i \setminus S) > 0
\]
where the last inequality follows from the assumption \(U_i \cap T \neq U_i\) and the fact that \(f(X) > 0\) unless \(X \in \mathcal{U}\) by the definition of \(f\) (recall (23)). Similarly,
\[
g(X \cap S) = g((S \triangle U_i) \cap U_i) = g(S \setminus U_i) = f((S \setminus U_i) \triangle S) = f(S \setminus (S \setminus U_i)) = f(S \cap U_i)
\]
> 0
holds where the last inequality follows from the assumption \(S \cap U_i \neq \emptyset\). Thus,
\[
\Phi_g(X, S) = g(X) + g(S) - g(X \cup S) - g(X \cap S) < 0
\]
holds, and we obtain the claim. \(\square\)
B Supplement to Section 3.4.5

This section shows the connection between the connected components of the inequality graph $G_f$ given in Section 3.3 and the inseparable decomposition (cf. [2, 15, 11, 5, 6]) for submodular functions. Precisely, we show the following.

**Proposition B.1.** Let $f : \{0, 1\}^V \to \mathbb{R}$ be a submodular function. For any set $U \subseteq V$, $\Phi_f(U, \overline{U}) = 0$ holds if and only if $U$ and $\overline{U}$ are disconnected in the inequality graph $G_f$, where $\overline{U} = V \setminus U$.

Notice that Proposition B.1 implies that $U_1, \ldots, U_k$ are inseparable decomposition of $f$ if and only if each $U_i$ is a connected component of $G_f$. As a preliminary step of the proof of Proposition B.1, we prove a simpler version of (25) in Theorem 3.13 in an elemental way comparing with [2, 1, 5] which considered the baseplytope.

**Theorem B.2 ([2]).** Let $\rho : \{0, 1\}^V \to \mathbb{R}$ be a submodular function satisfying that $\rho(\emptyset) = 0$. Suppose for $U \subset V (U \neq \emptyset)$ that $\rho(V) = \rho(U) + \rho(U)$ holds where $\overline{U} = V \setminus U$. Then,

$$\rho(X) = \rho(X \cap U) + \rho(X \cap \overline{U})$$

(40)

holds for any $X \in \{0, 1\}^V$.

**Proof.** To begin with, we remark that (40) is trivial for $X$ satisfying $X \subseteq U$ or $X \subseteq \overline{U}$. Thus, we prove (40) for $X$ satisfying both $X \cap U \neq \emptyset$ and $X \cap \overline{U} \neq \emptyset$. Since $\rho$ is submodular and $\rho(\emptyset) = 0$,

$$\rho(X) \leq \rho(X \cap U) + \rho(X \cap \overline{U})$$

(41)

$$\rho(X) \leq \rho(X \cup U) + \rho(X \cap \overline{U})$$

(42)

$$\rho(X) \leq \rho(X \cup \overline{U}) + \rho(X \cap U)$$

(43)

$$\rho(V) + \rho(X) \leq \rho(X \cup U) + \rho(X \cup \overline{U})$$

(44)

hold, respectively. By summing up (42), (43) and (44), we obtain that

$$\rho(X \cap U) + \rho(X \cap \overline{U}) \leq \rho(X)$$

(45)

holds, where we used the hypothesis that $\rho(V) = \rho(U) + \rho(U)$. Now, (41) and (45) imply (40).

As a corollary of Theorem B.2, we obtain the following.

**Corollary B.3.** Let $f : \{0, 1\}^V \to \mathbb{R}$ be a submodular function (and $f(\emptyset) = 0$ may not hold). Suppose for $U \subset V (U \neq \emptyset)$ that $f(V) + f(\emptyset) = f(U) + f(U)$ holds where $\overline{U} = V \setminus U$. Then,

$$f(X) + f(\emptyset) = f(X \cap U) + f(X \cap \overline{U})$$

(46)

holds for any $X \in \{0, 1\}^V$.

**Proof.** Let $\rho(X) = f(X) - f(\emptyset)$ for any $X \in \{0, 1\}^V$, then $\rho$ satisfies the hypothesis of Theorem B.2. Notice that $f(X) = \rho(X) + f(\emptyset)$ holds for any $X \in \{0, 1\}^V$. Thus, (40) implies (46).

Now we prove Proposition B.1.
Proof of Proposition B.1

(⇒) Suppose that $U$ and $\overline{U}$ are disconnected in $G_f$. Then, we prove

$$f(X) + f(\emptyset) = f(X \cap U) + f(X \cap \overline{U})$$

(47)

holds for any $X \in \{0, 1\}^V$, by an induction of the size $|X|$. Notice that (47) is trivial for $|X| = 0$ and $|X| = 1$. Inductively assuming that (47) holds for any $Y \in \{0, 1\}^V$ satisfying $|Y| \leq k$, we prove (47) for any $X \in \{0, 1\}^V$ satisfying $|X| = k + 1$. Notice that (47) is trivial if $X \subseteq U$ or $X \subseteq \overline{U}$, and we assume that $X \cap U \neq \emptyset$ and $X \cap \overline{U} \neq \emptyset$. Let $u \in X \cap U$, $v \in X \cap \overline{U}$, and $X' = X \setminus \{u, v\}$. Since $\{u, v\} \in E_f$,

$$f(X' \cup \{u\} \cup \{v\}) + f(X') = f(X' \cup \{u\}) + f(X' \cup \{v\})$$

(48)

holds. By the induction hypothesis, we obtain that

$$f(X' \cup \{u\}) + f(\emptyset) = f((X' \cup \{u\}) \cap U) + f(X' \cap \overline{U})$$

(49)

$$f(X' \cup \{v\}) + f(\emptyset) = f(X' \cap U) + f((X' \cup \{v\}) \cap \overline{U})$$

(50)

hold, as well as

$$f(X' \cap U) + f(X' \cap \overline{U}) = f(X') + f(\emptyset)$$

(51)

holds. By summing up (48)–(51), we obtain

$$f((X' \cup \{u\}) \cup \{v\}) + f(\emptyset) = f((X' \cup \{u\}) \cap U) + f((X' \cup \{v\}) \cap \overline{U}),$$

which implies (47) holds for the $X$. Let $X = V$, then we obtain the claim.

(⇒) Suppose $f(U) + f(\overline{U}) = f(V) + f(\emptyset)$ holds. Assume for a contradiction that there is a pair $u \in U$ and $v \in \overline{U}$ such that $\{u, v\} \in E_f$. This means that there is $X \subseteq V \setminus \{u, v\}$ such that $\Phi_f(X, \{u, v\}) \neq 0$ holds, by the definition (21) of $E_f$. For convenience, let $A = X \cap U$ and let $B = X \cap \overline{U}$ (see Figure 4). By Corollary B.3

$$f(X \cup \{u\}) + f(\emptyset) = f(A \cup \{u\}) + f(B)$$

(52)

$$f(X \cup \{v\}) + f(\emptyset) = f(A) + f(B \cup \{v\})$$

(53)

$$f(X \cup \{u, v\}) + f(\emptyset) = f(A \cup \{u\}) + f(B \cup \{v\})$$

(54)

$$f(X) + f(\emptyset) = f(A) + f(B)$$

(55)

hold, respectively. Thus,

$$\Phi_f(X, \{u, v\}) = f(X \cup \{u\}) + f(X \cup \{v\}) - f(X \cup \{u, v\}) - f(X)$$

$$= f(A \cup \{u\}) + f(B) + f(A) + f(B \cup \{v\})$$

$$- (f(A \cup \{u\}) + f(B \cup \{v\})) - (f(A) + f(B))$$

(by (52)–(55))

$$= 0$$

holds, which contradicts to the assumption that $(X, \{u, v\}) \in P$ satisfies $\Phi_f(X, \{u, v\}) \neq 0$.  

\[\square\]