USO Polytope

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1 Introduction

A unique sink orientation is an orientation of the hypercube such that for each subcube, there exists a unique sink. It was originally proposed by Stickney and Watson [24] in order to study the linear complementarity problem, in which it is formulated as a digraph structure. Since then, increasing attention has been paid to it because it is highly related to other classical optimization problems. In [12], it is shown that a linear program defines a USO, and finding the unique sink in the hypercube exactly solve the programming.

Up to now, many efforts have been committed to understand the structure of the USO itself [22] [27], propose fine-grained algorithm to find the global unique sink of the hypercube [11], analyze its relation to different optimization schemes [16] and other numerous aspects. Nonetheless, the relation between different USOs has not been discussed a lot and only little knowledge is known yet about the universal set of all possible USOs, likewise the estimation of the number of fixed points regard to the isomorphism transformation, or what implication can be learned from finding the unique sink in a similar USO. Therefore, we try to aggregate all possible USOs together to formulate the USO polytope, of which each vertex is a single USO. In this paper, we propose several aspects to analyze the structure of the USO polytope, both locally and globally, which will better our understanding of the relationship between different USOs.

Unique Sink Orientation. Since the formal introduction of Unique sink orientation in [22], it has been found of significant importance since many specific optimization problem can be reduced to find the unique sink in USOs, including P-matrix linear complementarity problem [24] and convex quadratic programming [14]. Therefore, it is fundamental to efficiently find the unique sink of USO. However, the complexity of the problem remains an open question, the best known algorithm for general USOs in [22] takes exponential number of queries . [21] provides us an almost quadratic lower bound for the general case while [10] offers an expected sub-exponential upper bound for the acyclic USOs.

Apart from finding the unique sink, there also exist many open questions for understanding the structure of USO. [18] proposes an estimation for the number of USOs and [7] estimates number of the number of P-matrix USOs. Besides, in terms of the construction of USOs, [3] finds a universal construction based on the periodic tilings and [9] proves that for each vertex of the D-cude, its L-graph is acyclic.

Although much attention is paid at specific USOs, in this paper, we take all the general USOs into consideration as a polytope, whose vertices are the USOs. In such a way we can leverage much knowledge in combinatorial geometry and polyhedral combinatorics.

Combinatorial Geometry. This topic usually deals with combinations and arrangements of geometric objects and their discrete combinatorial properties. Since it was introduced by Hadwiger, Debrunner and Klee [13] in 1955, it has been so far developed to an extent which is involved with topology, graph theory, combinatorial optimization and many other aspects. Some significant results include [15] which shows a counterexample to Borsuk's conjecture [2] in certain high dimension, [20] which proves the Sylvester-Gallai Theorem [26].

Polyhedral Combinatorics. Topics in this area usually studies the problems of describing the faces of the convex polytope, accessing the combinatorial property of the polytope graph, and also application of the theory of polyhedron and linear systems to combinatorics. An interesting problem among these is counting the number of the faces and [19] proves that asymptotically, there are at most $n^{\lfloor d/2 \rfloor}$ faces for d-dimensional polytope with n vertices. Another important topic in this area falls on the 0/1-polytope, which is indeed the USO polytope belongs to, and [1] proves that each Birkhoff polytope (a subclass of 0/1-polytope) can be described as two types of linear inequality or equality.

In our paper, particularly, we cares more about the combinatorial meaning of the faces and symmetry group of the USO polytope.

Organization of the Paper We give some basic definitions and background knowledge about USO and polytopes in section 2, including some lemmas achieved by us. Next, we properly define the USO polytope in section 3 and introduce some necessary knowledge about the 0/1 polytope. Based on that, we try to understanding the combinatorial meaning and structure of the USO polytope both locally and globally, by analyzing the faces and isometry of the polytope. Finally, we conclude this paper with several open conjectures and potential directions in the future in section 4.

Main Results

- Lemma 7 and 8, argument about the structure of outmap and a sufficient condition for a subcube to be flippable.
- Lemma 13, Corollary 15 and Algorithm 1, theoretical and empirical analysis about the structure of USO polytope.
- Lemma 21 and 22, argument about USO isomorphism and a sufficient condition for it to admit non zero fixed points.
- Theorem 24 and 28, necessary and sufficient condition for general polytope isomorphism and USO polytope automorphism.

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2 USO

2.1 Definition

The following definitions about USO are adapted from section 2 in [22], and some notations may differ.

2.1.1 Hypercube

Definition 1. *The hypercube of dimension n is an undirected graph denoted as Q_n. The vertex set is $V(Q_n) = 2^{[n]}$, and the edge set is $E(Q_n) = \{\{u,v\}||u \oplus v| = 1\}$, where $\oplus$ denotes the symmetric set difference.*

The coordinate of vertex u is characterized by e_u, where

$$[e_u]_i = \begin{cases} 1, & i \in u, \\ 0, & i \notin u. \end{cases}$$

Another alternative notation for hypercube is in 0/1-words. A 0/1-word of length n is $u = (u_0, u_1, \cdots, u_{n-1}) \in \{0,1\}^n$. The vertex set $V(Q_n) = \{0,1\}^n$ and the edge set $E(Q_n) = \{\{u,v\} \,|d_H(u,v) = 1\}$, where $d_H(u,v) = k$ if and only if they differ in exact k positions.

Definition 2. *A subcube P of Q_n can be characterized by its corner u and direction A. Denote the subcube anchored at u and spanned in set of directions $A \subseteq [n]$ as $P(u,A)$. Accordingly,*

$$V(P(u,A)) = \{u \oplus v | v \subseteq A\}.$$

For simplicity, we can assume that $u \cap A = \varnothing$, since as long as $u \setminus A = v \setminus A$, we have $P(u,A) = P(v,A)$.

Another alternative way to characterize a subcube R of Q_n is via its minimal vertex u and maximal vertex v such that $u \subseteq v$, where

$$R(u,v) = \{w | u \subseteq w \subseteq v\}.$$

Generally, the minimal subcube that covers the vertex set U is $R(\cap_{v \in U} v, \cup_{v \in U} v)$, which is called the subcube spanned by the vertex set U.

2.1.2 Unique Sink Orientation

Definition 3. *A unique sink orientation s of Q_n is an orientation of $E(Q_n)$ such that each subcube of Q_n has a unique sink. Let Ψ be the set of directed edges in s. For all $e = \{u,v\} \in E(Q_n), [(u,v) \in \Psi] \oplus [(v,u) \in \Psi]$.*

A USO s can be characterized by its outmap function $S : 2^{[n]} \to 2^{[n]}$, where

$$S(u) = \{\lambda | (u, u \oplus \{\lambda\}) \in \Psi\}.$$

.

For each edge $e = \{u, v\}$ in the orientation s of the hypercube Q_n, the orientation indicator $I_s(u, v)$ is defined by

$$I_s(u, v) = \begin{cases} 1, & (u, v) \in \Psi, \\ 0, & (v, u) \in \Psi. \end{cases}$$

In orientations indicator words, we can alternatively define outmap $S(u)$ as

$$S(u) = \{\lambda | I_s(u, u \oplus \{\lambda\}) = 1\}.$$

Remark. In the following context, we use (u, v) to denote the undirected edge $\{u, v\}$ or the directed edge (u, v) from u to v if the orientation is specified.

2.1.3 Phase

Definition 4. *An edge $e = (u, v)$ is called λ-edge if $u \oplus v = \{\lambda\}$. Two different λ-edges e_1, e_2 are called in direct phase, denoted by $e_1 \| e_2$, (definition 4.7 in [22]) if there exists $u \in e_1, v \in e_2$, such that*

$$(u \oplus v) \cap (S(u) \oplus S(v)) = \{\lambda\}.$$

Specifically, for any edge e, we define $e \| e$, implying that $\|$ is reflexive and symmetric. Let $\sim$ be the transitive closure of $\|$, which is an equivalence relation. $\phi(e)$ is called the phase of edge e, and $\phi(e) = \{e' | e' \sim e\}$. A phase of a λ-edge is called λ-phase.

For more detail about the structure of USO, see section 4 in [22].

2.1.4 Polytope

The following concepts and notations about polytopes are adapted from chapter 2 in [4].

Definition 5. *Let $x_i \in X \subseteq R^n, \lambda_i \in R, i \in [k]$, then the linear combination $\sum_{i=1}^{k} \lambda_i x_i$ is called convex combination of X if*

(i) $\forall i \in [k], \lambda_i \geq 0$.

(ii) $\sum_{i=1}^{k} \lambda_i = 1$.

A linear combination $\sum_{i=1}^{k} \lambda_i x_i$ is called a conic combination if it fulfills

(i) and an affine combination if it fulfills (ii).

Definition 6. *Let $X \subseteq R^n$. Then*

- *the affine hull $affn(X)$, is the set of all affine combination of X.*
- *the conic hull $cone(X)$, is the set of all conic combination of X.*
- *the convex hull $conv(X)$, is the set of of all convex combination of X.*

By definition, it is clear that $conv(X) = affn(X) \cap cone(X)$. Thus, we can define the dimension of a point set X regard to its affine hull $affn(X)$.

Definition 7. *The dimension of a point set $X \in R^{n \times k}$, denoted as $dim(X)$, is determined by its affine hull $y = affn(X)$,*

$$dim(X) = \min\{k \in \mathbf{N} : \exists A \in R^{n \times n}, rank(A) = n - k, \forall x, y \in X, Ax = Ay\}.$$

In other words, if there exists a matrix A with rank at least $n-k$, and $\forall x, y \in X$, we have $x - y \in ker(A)$, it is implied that X has dimension as most k.

Definition 8. *Let $w \in R^n \setminus \{0\}$ and $b \in R^n$. Then the $n-1$ dimensional subspace $H_{w,b} = \{w^\top x + b = 0\}$ is called a hyperplane of R^n.*

Accordingly, a hyperplane $H_{w,b}$ defines a positive half-space H^+ and a negative half-space H^- respectively:

- $H^+ = \{x \in R^n | w^\top x + b \geq 0\}$
- $H^- = \{x \in R^n | w^\top x + b \leq 0\}$

Definition 9. *Let $A \in R^{m \times n}$ and $b \in R^m$, the set $P = \{x \in R^n | Ax \leq b\}$ is called a polyhedron, and a bounded polyhedron is called a polytope.*

As it is defined, a polytope can be regarded as the intersection of finite many half-spaces.

Remark. Without specification, in the following sections, we always talk about nonempty and bounded polyhedron.

Definition 10. *Let P be a polyhedron, a hyperplane H is called as a supporting hyperplane of P if $P \cap H \neq \varnothing$, and either $P \subseteq H^+$ or $P \subseteq H^-$.*

Specifically, for a supporting hyperplane H and $x, y \in P$, if $x \in P \cap H$ and $y \notin P \cap H$, we say that H supports P on x and excludes y respectively.

Definition 11. *Let $P \subseteq R^n$ be a polyhedron and $dim(P) > 0$, a d-dimensional face f with $dim(f) = d$ is either P itself, the empty set or the intersection of P and some supporting hyperplane H. Hence, f is called*

- *a vertex, if f is a 0-dimensional face.*
- *an edge, if f is a 1-dimensional face.*
- *a facet, if f is a $(dim(P) - 1)$-dimensional face.*

Specifically, an empty set $\varnothing$ is regarded as a (-1)-face. By definition, to validate either f is a face of P, it is equivalent to validate whether there exist a supporting hyperplane H such that H supports P on f and excludes any other points.

We conclude the definitions about polytope by the following lemma.

Lemma 1. *Let $X \subseteq R^n$ be a set of points in R^n, $P = conv(X)$. Let $X' \subseteq X, S = X \cap conv(X'), T = X \setminus T$ and $S \neq \varnothing$, $T \neq \varnothing$. Then $conv(S)$ is a face of P if and only if there exist a hyperplane $H_{w,b}$: $\{x|f(x) = w^\top x + b = 0\}$, such that $\forall x \in S, f(x) = 0$ and $\forall x \in T, f(x) > 0$.*

Proof. "$\Rightarrow$": Suppose that $conv(S)$ is a face of P, then there exists H such that $P \cap H = conv(S)$ and $P \subseteq H^+$, and hence $T \subseteq H^+$. Notice that $T \cap conv(S) = \varnothing$, thus $T \cap H = \varnothing$. Therefore, $\forall x \in S, x \in conv(S) \subseteq H$, $f(x) = 0$. Hence, $\forall x \in T$, $x \notin H$, $x \in H^+ \setminus H$, and $f(x) > 0$.

"$\Leftarrow$": Suppose that there exist such hyperplane H, and we will prove that $H \cap P = conv(S)$ and $P \subseteq H^+$, indicating that $conv(S)$ is a face of P.

First we argue that $P \subseteq H^+$. $\forall y \in P$, it is a convex combination of X, and $y = \sum_i \lambda_i x_i$. Therefore,

$$\begin{aligned} f(y) &= w^\top y + b \\ &= w^\top (\sum_i \lambda_i x_i) + b \\ &\overset{(a)}{=} w^\top (\sum_i \lambda_i x_i) + (\sum_i \lambda_i b) \\ &= \sum_i \lambda_i f(x) \overset{(b)}{\geq} 0, \end{aligned}$$

where (a) stands for $\sum_i \lambda_i = 1$, and (b) holds because $\forall i, f(x_i) \geq 0$ and $\lambda_i \geq 0$, implying that $P \subseteq H^+$.

Next we argue that $H \cap P = conv(S)$. $\forall y \in conv(S)$, analogous to the above equation, we have $f(y) = 0$ and $y \in H$. $\forall x \in P \setminus conv(S)$, $y = \sum_i \lambda_i x_i$. Notice that $y \notin conv(S)$, there exist k such that $x_k \in T$ and $\lambda_k > 0$. Therefore,

$$f(y) \geq \lambda_k f(x_k) > 0,$$

implying that $(P \setminus conv(S)) \cap H = 0$, and $H \cap P = conv(S)$. Combined with $P \subseteq H^+$, we conclude that $conv(S)$ is a face of P. □

REMARK. The polytope P itself and the null-face $\varnothing$ are also regarded as faces of P, which are not the intersection of P and supporting hyperplane H, and also do not belong to the cases that Lemma 1 can apply.

2.2 Structure of USO

Lemma 2. *Let S be the outmap of the USO s of Q_n. Let $A \subseteq [n]$, $[S \oplus A](u) := S(u) \oplus A$. $S \oplus A$ is an outmap of the orientation which flips the edges in the directions of A and it is also a USO outmap.*

PROOF. See Lemma 4.1 in [22].

Lemma 3. *Let S_Q be the outmap of the USO s of Q_n. For any subcube $P(u, A)$ of Q_n, the outmap restricted on it is $S_P(v) = S_Q(v) \cap A$, which is bijective.*

PROOF. See Lemma 4.1 in [22].

Corollary 4. *S is a outmap of a USO of hypercube Q_n, then S is a bijection from $2^{[n]}$ to $2^{[n]}$.*

PROOF. See Corollary 4.2 in [22].

Lemma 2 shows that the outmap is bijective on any subcube. Combined with Corollary 3, it implies that a unique sink orientation is also a unique source orientation. In other words, each subcube has an unique source whose incident edges are all directed outgoing.

Lemma 5. *S is a outmap of a USO if and only if for any different u and v, $(S(u) \oplus S(v)) \cap (u \oplus v) \neq \varnothing$.*

PROOF. See Proposition 4.3 in [22].

Lemma 6. *For any set of directions A and USO outmap S_Q, the A-sink-inherit outmap (see section 3 in [27]) $S_{Q/A}(u), u \cap A = \varnothing$ is defined by $S_{Q/A}(u) = S_Q(v) \setminus A$, where v is the unique sink in the subcube $P(u, A)$. Hence, $S_{Q/A}$ is another USO outmap with $|A|$ dimensions lower.*

Similarly, the A-source-inherit outmap $S_{Q/A}(u), u \cap A = \varnothing$ is defined by $S_{Q/A}(u) = S_Q(v) \setminus A$, where v is the unique source in the subcube $P(u, A)$.

Proof. See Lemma 3.1 in [27]. Here we provide an alternative proof which fits in our context.

Since $S_{Q/A/B} = S_{Q/(A \cup B)}$, we can suppose that $|A| = 1$. First we will show that $S_{Q/A}$ is a valid outmap. In other words, $S(u)$ agrees with each other and each edge exists exactly once in the outmap of two endpoints, implying that

$$(S_{Q/A}(u) \cap d) \oplus (S_{Q/A}(v) \cap d) = d, \forall (u, v) \in Q_n/A,$$

where $d = u \oplus v$.

Consider the edge (u, v) in Q/A. There are two different cases.

- $I_Q(u, u \oplus A) = I_Q(v, v \oplus A)$. Suppose that $I_Q(u, u \oplus A) = I_Q(v, v \oplus A) = 0$, thus $S_{Q/A}(u) = S_Q(u), S_{Q/A}(v) = S_Q(v)$. Therefore, $(S_{Q/A}(u) \cap d) \oplus (S_{Q/A}(v) \cap d) = (S_Q(u) \cap d) \oplus (S_Q(v) \cap d) = d$.
- $I_Q(u, u \oplus A) \neq I_Q(v, v \oplus A)$. Suppose that $I_Q(u, u \oplus A) = 0$ and $I_Q(v, v \oplus A) = 1$. Notice that $(u, v, u \oplus A, v \oplus A)$ is a USO, implying $I_Q(u, v) = I_Q(u \oplus A, v \oplus A)$. Accordingly, $d \subseteq S_Q(u) \oplus S_Q(v \oplus A)$. Therefore, $(S_{Q/A}(u) \cap d) \oplus (S_{Q/A}(v) \cap d) = (S_Q(u) \cap d) \oplus (S_Q(v \oplus A) \cap d) = d$.

Next we will show that $S_{Q/A}$ is a USO outmap. It suffice to prove that there is a unique sink in $S_{Q/A}$. Suppose that $S_{Q/A}(u) = \varnothing$, thus $S_Q(v) \subseteq A$. Since v is the unique sink in $P(u, A)$, we have $S_Q(v) \cap A = \varnothing$. Accordingly, $S_Q(v) = \varnothing$, v is also the unique sink of Q and $S_{Q/A}$ is a USO outmap. $\square$

This lemma shows what a USO outmap S is composed of. Instead of naturally dividing Q_n into to subcube $P(\varnothing, [n-1])$ and $P(\{n\}, [n-1])$, we can also take $A = \{n\}$ and compress S into a sink-inherit outmap and a source-inherit outmap with regard to the direction A.

Lemma 7. *Let s be a USO of Q_n and S be its outmap. Define $f_S(u) = u \oplus S(u)$ and $f_S^{-1}(x) = \{u | f_S(u) = x\}$. For any $x \in Q_n$, we claim $|f_S^{-1}(x)|$ is even.*

Proof. We prove this by induction. It is clear that this statement holds for Q_1. Suppose that for Q_{n-1} this claim holds. Take $A = \{n\}$ and consider the outmaps restricted on the subcubes $P(\varnothing, [n-1])$, $P(\{n\}, [n-1])$ and the A-sink-inherit outmap. We introduce two auxiliary function,

$$g_S^{-1}(x) = \{u | f_S(u) = x \wedge n \notin u\},$$
$$h_S^{-1}(x) = \{u | f_S(u) = x \wedge n \in u\},$$

and it is clear that $|f_S^{-1}(x)| = |g_S^{-1}(x)| + |h_S^{-1}(x)|$. Actually, g_S^{-1} and h_S^{-1} is a partition of the f_S^{-1} based on where the preimage u comes from.

Consider two disjoint subcubes $P_1 = P(\varnothing, [n-1])$ and $P_2 = P(\{n\}, [n-1])$. Denote the restricted outmap as $S_1(u)$ and $S_2(u)$ respectively. Therefore,

$$S_1(u) = S(u) \cap [n-1], f_{S_1}(u) = u \oplus S_1(u),$$
$$S_2(u) = S(u) \cap [n-1], f_{S_2}(u) = u \oplus S_2(u).$$

According to the induction, $|f_{S_1}^{-1}(x)|$ and $|f_{S_2}^{-1}(x)|$ are both even. Notice that $\forall u \in P_1$, either $S(u) = S_1(u)$ or $S(u) = S_1(u) \cup \{n\}$. Therefore, $f_{S_1}(u) = f_S(u)$ or $f_{S_1}(u) = f_S(u) \cup \{n\}$, indicating that $\forall x \subseteq [n-1]$,

$$|g_S^{-1}(x)| + |g_S^{-1}(x \cup \{n\})| \equiv 0 \pmod 2. \tag{1}$$

Analogous to (1), we have $f_{S_1}(u) = f_S(u)$ or $f_{S_1}(u) \cup \{n\} = f_S(u)$, and then

$$|h_S^{-1}(x)| + |h_S^{-1}(x \cup \{n\})| \equiv 0 \pmod 2. \tag{2}$$

Let $A = \{n\}$ and consider the A-sink-inherit outmap $S_3 = S_{Q/A}$. Since $S_3(u) = S_Q(v) \setminus \{n\}$ and v is the unique sink in $P(u, \{n\})$, $n \notin S_Q(v)$, we have $S_3(u) = S(v), f_{S_3}(u) = f_S(v) \oplus (u \oplus v)$. According to the induction, we have $|f_{S_3}^{-1}(x)|$ is even. Notice that $u \oplus v \in \{\varnothing, \{n\}\}$, thus, $\forall x \subseteq [n-1]$,

$$|g_S^{-1}(x)| + |h_S^{-1}(x \cup \{n\})| \equiv 0 \pmod 2. \tag{3}$$

(1) + (3):

$$|g_S^{-1}(x \cup \{n\})| + |h_S^{-1}(x \cup \{n\})| \equiv 0 \pmod 2. \tag{4}$$

(2) + (3):

$$|g_S^{-1}(x)| + |h_S^{-1}(x)| \equiv 0 \pmod 2. \tag{5}$$

Therefore, $\forall x \in Q_n$, we have

$$|f_S^{-1}(x)| = |g_S^{-1}(x)| + |h_S^{-1}(x)| \equiv 0 \pmod 2,$$

implying that the statement also holds for Q_n, thus completing the induction. $\square$

Lemma 8. *Let s be a USO of Q_n and S be its outmap. Suppose that there exists a subcube $P(w, A) \subseteq Q_n$ such that for any vertex $u, v \in P(w, A)$, we have $u \oplus S(u) = v \oplus S(v)$. Then, the orientation s' obtained by flipping each edge in $P(w, A)$ from s is another USO.*

Proof. To see this, first we need to argue that s restricted on $P(w, A)$ is a uniform USO. A uniform USO is an orientation such that for any λ, each λ-edge shares the same orientation.

The outmap restricted on the subcube $P(w, A)$ is $S_P(u) = S_Q(u) \cap A$. For any edge $e = (u, v)$, the orientation indicator is

$$I_s(u, v) = |S(u) \cap (u \oplus v)|.$$

Therefore, for any two λ-edge $e_1 = (u_1, v_1), e_2 = (u_2, v_2), u_1 \subseteq v_1, u_2 \subseteq v_2$, we have

$$I_s(u_1, v_1) = |S(u_1) \cap \{\lambda\}|,$$
$$I_s(u_2, v_2) = |S(u_2) \cap \{\lambda\}|.$$

Notice that $S(u_1) \oplus u_1 = S(u_2) \oplus u_2$ and $u_1 \cap \{\lambda\} = u_2 \cap \{\lambda\} = \varnothing$, we have $S(u_1) \cap \{\lambda\} = S(u_2) \cap \{\lambda\}$, indicating that $I_s(u_1, v_1) = I_s(u_2, v_2)$. Actually, for any uniform USO s, its outmap S can be characterized by its unique sink t such that $\forall u, S(u) = u \oplus t \oplus S(t)$.

Next we need to argue that for any subcube $P(u, B)$ in the orientation s', it has a unique sink. Let S' be the outmap of orientation s'. There are following several cases to consider.

- $P(u, B) \cap P(w, A) = \varnothing$. Accordingly, the orientation of $P(u, B)$ in s' remains the same as in s, indicating that the sink is unique.
- $P(u, B) \cap P(w, A) = C \neq \varnothing$. For any $v \in C$, notice that $S'(v) = S(v) \oplus A$ and $S(v) = S(t) \oplus (v \oplus t)$, where t is the unique sink in $P(w, A)$. Thus, $S'(v) = S(t) \oplus t \oplus v \oplus A$. Notice that $t \oplus v \subseteq A$, then $t \oplus v \oplus A \subseteq A$. Consider the unique sink of the subcube $P(u, B)$ in the orientation s'. We can distinguish the following two cases:
  - $B \cap (S(t) \setminus A) \neq \varnothing$. Then for each vertex $v \in C$, we have $S(v) \cap B \neq \varnothing$ and $S'(v) \cap B \neq \varnothing$, indicating that each vertex in C is neither a sink of $P(u, B)$ in s nor in s'. Then, the original unique source in $P(u, B)$ remains the same.
  - $B \cap (S(t) \setminus A) = \varnothing$. Then for each vertex $v \in C$, we have $(S(v) \setminus A) \cap B = \varnothing$ and $(S'(v) \setminus A) \cap B = \varnothing$, indicating that each vertex in C has no edge directed out of C in $P(u, B)$. Therefore, the unique sink of C is exactly the unique sink of $P(u, B)$.

In all the cases discussed above, each subcube $P(u, B)$ has a unique sink, indicating that s' is another USO. □

Remark. Specifically, for any outmap S of a USO, if there exists an edge $e = (u, v)$ such that $u \oplus S(u) = v \oplus S(v)$, then flipping the edge e will transform

s into another USO s'. One may conjecture that for any USO s, such edge always exists. As it is shown in Lemma 7, $\forall u \in Q_n$, there exist v other than u such that $u \oplus S(u) = v \oplus S(v)$. However, it is not the case that there always exists such adjacent u and v, and [17] implicitly shows a counter example in dimension eight with a tiling of unit cubes. Generally, whether we can flip some edges in a USO to get another USO is closely related to phases, which will be illustrated in detail next.

Fact 9. *Let s be a USO and λ-edges e_1 and e_2 are in direct phase. Another orientation s' is obtained by only flipping e_1 in s and s' is not a USO.*

Proof. See definition 4.7 in [22].

This fact implies that, in order to flip some specific λ-edge e to get another USO, it is necessary to flip all the edges in the phase of e or some edges adjacent to the edge e.

Lemma 10. *Let s be a USO and let L be a set of non-adjacent edges in s, essentially a matching. Flipping all the edges in L transforms s into the orientation s', and s' is also a USO if and only if L is a union of phase(s).*

Proof. See Proposition 4.9 in [22].

3 USO Polytope

3.1 Definition

Let $E(Q_n) = (\{u_1, v_1\}, \{u_2, v_2\}, \cdots, \{u_m, v_m\}\})$ be an ordered sequence of the edges and $m = n2^{n-1}$. Let us fix an arrangement of the edges such that for any λ_1-edge $e_1 = (u_1, v_1)$ and λ_2-edge $e_2 = (u_2, v_2)$, e_1 appears before e_2 in $E(Q_n)$ if either of the following happens:

- $\lambda_1 < \lambda_2$,
- $\lambda_1 = \lambda_2 \wedge O(u_1) < O(u_2)$,

where $O(u) : 2^{[n]} \to \mathbb{N}$ implies a total order on $2^{[n]}$ and $O(u) = \sum_{i=1}^{n} 2^i [i \in u]$.

USO s of Q_n can be represented by its USO vector $p_s \in \{0,1\}^{n2^{n-1}}$. For the i-th edge $e_i = (u_i, v_i)$ in $E(Q_n)$, we take

$$(p_s)_i = I_s(u_i, v_i), u_i \subseteq v_i.$$

Definition 12. *The USO polytope P_n is defined as the convex hull of p_s, $P_n = conv(p_s)$, where s is all the possible USO of Q_n.*

Actually, the USO polytope P_n is a special case of 0/1-polytope, of which some facts we will discuss next.

3.2 0/1 Polytope

Definition 13. *A d-dimensional 0/1 polytope P is the convex hull of d-dimensional 0/1 vector set X. In other words, $\forall x \in X, x = (x_1, x_2, \cdots, x_d)$, $x_i \in \{0,1\}$ and $P = conv(X)$.*

Alternatively, we can describe each $x \in \{0,1\}^d$ with set words by the explicit mapping $f : \{0,1\}^d \to 2^{[d]}$, such that

$$f(x) = \{i | x_i = 1\}.$$

It is clear that f is bijective and its inverse f^{-1} is unique:

$$f^{-1}(y) = ([1 \in y], [2 \in y], \cdots, [d \in y]).$$

Analogous to the set operation, we can define the union and intersection operation for u and v in $\{0,1\}^d$:

$$u \cup v = f^{-1}(f(u) \cup f(v)),$$
$$u \cap v = f^{-1}(f(u) \cap f(v)),$$
$$u \oplus v = f^{-1}(f(u) \oplus f(v)).$$

For the corner $u \in \{0,1\}^d$ and direction $A \in \{0,1\}^d$ with $u + A \in \{0,1\}^d$, we define the subcube anchored at u as $P(u, A)$,

$$P(u, A) = \{u + v | f(v) \subseteq f(A)\}$$

For u and v with $f(u) \subseteq f(v)$, the minimum subcube covering u and v is defined as $R(u, v)$,

$$R(u, v) = \{w | f(u) \subseteq f(w) \subseteq f(v)\}.$$

For any set X, the minimum subcube that covers the convex hull of X is $R(\cap_{x \in X} x, \cup_{x \in X} x)$.

For simplicity, we define $u \subseteq v$ if and only if $f(u) \subseteq f(v)$. Similarly, we omit f and f^{-1} and use the set words and 0/1-vector words interchangeably in following sections when the case is clear.

3.2.1 Vertex of 0/1 Polytope

Fact 11. *Let $P = conv(X)$ and $X \subseteq \{0,1\}^d$. Then, $\forall x \in X$, x is an extreme point (0-face) of P.*

Proof. For $x \in X$, consider the hyperplane $h(y) = (\mathbf{1} - 2x)^\top y + x^\top x = 0$. Notice that

$$\begin{aligned} h(y) &= \sum_i (y_i - 2y_i x_i + x_i^2) \\ &\overset{(a)}{=} \sum_i (y_i - x_i)^2 \geq 0, \end{aligned}$$

where (a) stands because $y_i \in \{0,1\}$ and $y_i = y_i^2$. Therefore, $h(y) = 0$ if and only if $y = x$ and the hyperplane $h(y) = 0$ only support the vertex x and excludes other points, implying that x is an extreme point. □

3.2.2 Edge of 0/1 Polytope

Fact 12. *Let $P = conv(X)$ and $X \subseteq \{0,1\}^d$. For $x, y \in X$, suppose that for the subcube $R(x \cap y, x \cup y)$, $X \cap R(x \cap y, x \cup y) = \{x, y\}$, then the segment $e = (x, y)$ is an edge (1-face) of P.*

Proof. To see this, take $u = x \cap y, v = x \cup y$. Consider the hyperplane $h(z) = (\mathbf{1} - u - v)^\top z + u^\top u = 0$. Notice that

$$\begin{aligned} h(z) &= \sum_i (z_i^2 - z_i u_i - z_i v_i + u_i^2) \\ &= \sum_i (z_i(z_i - v_i) + u_i(u_i - z_i)). \end{aligned}$$

Since $u_i \leq v_i$, there are two cases to consider.

- $u_i = v_i$, then $z_i(z_i - v_i) + u_i(u_i - z_i) \overset{(a)}{=} (z_i - u_i)^2 \geq 0$,
- $u_i = 0, v_i = 1$, then $z_i(z_i - v_i) + u_i(u_i - z_i) \overset{(b)}{=} z_i(z_i - 1) = 0$,

where (a) and (b) hold since $z_i \in \{0, 1\}$.

Therefore, $h(z) = 0$ if and only if $u \subseteq z \subseteq v$, indicating that $z \in R(u, v)$. Notice that x and y are the only two vertex inside $R(u, v)$. The hyperplane $h(z) = 0$ only supports vertices x, y and excludes other vertices, thus making $e = (x, y)$ a 1-face of P. □

Lemma 13. *Let $X \subseteq \{0, 1\}^d$. For any segment $e = (x, y), x, y \in X$ and the subcube $R(u, v)$ spanned by it, where $u = x \cap y, v = x \cup y$, let $X' = X \cap R(u, v)$. The segment $e = (x, y)$ is an edge of $conv(X)$ if and only if it is an edge of $conv(X')$.*

PROOF. $\Rightarrow$: Necessity is oblivious. Suppose that $e = (x, y)$ is an edge of $conv(X)$, there exists a hyperplane $h(z) = 0$ which only support vertices x and y in X. Since $X' \subseteq X$, $h(z) = 0$ is also the supporting hyperplane of $conv(X')$ on x and y, implying that $e = (x, y)$ is the edge of $conv(X')$.

$\Leftarrow$: To see sufficiency, suppose that $e = (x, y)$ is an edge of $conv(X')$. Denote $A = u \oplus v$. There exists a hyperplane $h_1(z) = w^\top z + b = 0$ such that

$$\begin{gathered} h_1(x) = h_1(y) = 0 \\ \forall z \in X', z \neq x, z \neq y, h_1(z) > 0 \\ \forall i \notin A, w_i = 0. \end{gathered}$$

Therefore, for any $x \in X$, we have $h_1(z) = h(z \cap A)$. Hence, consider the hyperplane $h_2(z) = t^\top(z - u)$, where $t_i = C/(1 - 2u_i)$ for $i \notin A$. Then, for any z, we have $h_2(z) = t^\top(z - u) = Cd_H(u, z \cap \overline{A})$, where d_H is the Hamming distance and $\overline{A}$ is the complement set of A.

Thus, for any $z \in R(u, v)$, we have $u = z \cap \overline{A}$ and $h_2(z) = 0$. For any $z \notin R(u, v)$, we have $d_H(u, \cap \overline{A}) \geq 1$, thus implying $h_2(z) \geq C$.

Let $h_3(z) = h_1(z) + h_2(z)$. For $z \in R(u, v)$, we have $h_3(z) = h_1(z)$. For $z \notin R(u, v)$, we have $h_3(z) \geq h_1(z) + C$. Since X is finite, there exist sufficient large constant C, such that $h_3(z) > 0$ for $z \notin R(u, v)$.

Combine the above, it is clear that $h_3(z) = 0$ supports X only on the point x and y, which means that $e = (x, y)$ is also an edge of $conv(X)$. □

Generally, this lemma implies strong locality. In other words, to determine whether a segment is an edge of the polytope, it suffices to only inspect the subcube of spanned by the endpoints.

3.3 Polytope Graph

Definition 14. *For any polytope P, its polytope graph G is defined as $G = (V, E)$, where V is the set of extreme points of P and $(u, v) \in E$ if and only if it is an edge (1-face) of P.*

The polytope graph is an abstraction of the polytope by connecting the vertices with the edges of the polytope.

Specifically, for each edge $e \in E$, we define $w(e) = d_H(u, v)$, where $w(e)$ is the distance/weight of the edge e and $d_H(u, v) = |u \oplus v|$ is the Hamming distance.

Lemma 14. *Let G be the polytope graph of a 0/1 polytope P and $d_G(u, v)$ denote the length of shortest path between u and v in G, then we have $d_G(u, v) = d_H(u, v)$.*

Proof. We prove this by induction.

Let $m = d_H(u, v)$. Take $m = 0$, we have $d_H(u, v) = 0 \implies u = v$, and the claim stands clearly.

Take $m = 1$, we have $d_H(u, v) = 1$. Notice that (u, v) is the edge of the hypercube. Therefore, (u, v) is also the edge of any 0/1 polytope that includes vertices u and v, $(u, v) \in E$ and $d_G(u, v) = w(e) = d_H(u, v)$. The claim also stands.

Suppose that the claim stands for any $m \in [0, k]$. Take $m = k + 1$. For any (u, v) with $d_H(u, v) = k + 1$, let $X' = R(u \cap v, u \cup v)$ and G' be the polytope graph of $conv(X')$. According to Lemma 13, G' is a subgraph of G, indicating that for any (u, v), $d_G(u, v) \leq d_{G'}(u, v)$.

Take any vertex t such that w is adjacent to u in G'. Since $t \in R(u \cap v, u \cup v)$, we have $d_H(u, t) + d_H(t, v) = d_H(u, v)$. Hence, by induction we have $d_{G'}(t, v) = d_H(t, v)$ and $d_{G'}(u, t) = w(u, t) = d_H(u, t)$. Therefore, we have

$$\begin{aligned} d_G(u, v) &\leq d_G(u, t) + d_G(t, v) \\ &\leq d_{G'}(u, t) + d_{G'}(t, v) \\ &= d_H(u, t) + d_H(t, v) \\ &= d_H(u, v). \end{aligned}$$

Notice that by construction, we have $d_G(u, v) \geq d_H(u, v)$. Combine these together to get $d_G(u, v) = d_H(u, v)$, thus completing the induction. $\square$

Remark. Intuitively, this lemma implies that the shortest routing from u to v in the polytope graph G never takes detour. Essentially, for any u, v, there exist $w_1, w_2, \cdots, w_k \in 2^{[n]}$, such that

$$u \subseteq w_1 \subseteq \cdots w_i \subseteq w_{i+1} \subseteq \cdots w_k \subseteq v,$$
$$(u, w_1), (w_k, v), (w_i, w_{i+1}) \in E(G), \forall i \in [k-1],$$

and the chain $(u, w_1, \cdots, w_k, v)$ is a shortest path.

3.4 Computing USO Polytope

3.4.1 Computational Complexity

Though we properly define the USO polytope, actually, it is not feasible to compute all the faces of USO polytope, even for P_3. Given a d-dimensional polytope P with r vertices, the problem to compute all the facets for P is referred to as facet-enumeration. Typical schemes to solve this includes randomized incremental construction[6], gift-wrapping method[25] and shelling method[23]. However, as we have $O(r^{\lfloor d/2 \rfloor})$ face in P_n, and $r \in n^{2^{\Theta(n)}}$ for USO polytope P_n by [18], it is not feasible to compute all the faces of P_n in practice.

Alternatively, we will investigate the 0, 1, and 2-faces of P_n instead, in which we do not enumerate over all the faces and achieve affordable computational cost.

Remark. [28] shows that for a general 0/1-polytope, it might have exponential or super-exponential number of facets, while the number of faces in the USO polytope remains open. In the appendix, we provides some numerical estimation of the faces in P_3.

3.4.2 Vertex of USO polytope

Since P_n is a 0/1 polytope, each p_s is its vertex.

Proof. See Fact 11.

3.4.3 Edge of USO polytope

By 1, suppose that the segment (p_s, p_t) is a 1-face (edge), there exists a hyperplane which only supports vertex p_s, p_t and excludes other vertices. To verify this, we check the feasibility of the following linear system.

$$w^\top p_u + b \geq 1, \forall u \notin \{s, t\},$$
$$w^\top p_s + b = w^\top p_t + b = 0.$$

If the above LP is feasible, (p_s, p_t) is an edge. Otherwise, it is not.

A straight forward way to understand the combinatorial meaning of the edge (p_s, p_t) is that flipping set of edges L would transform the USO s into t, or vice versa. However, suppose that there are N different USOs, there are in total $\binom{N}{2}$ such flips. Not each such flips is an edge in P_n unless the USO Polytope is a simplex, which is not true.

Therefore, it raises a question that how can we distinguish edges and non-edges by their combinatorial meanings. Here we provide some sufficient conditions based on the phase decomposition.

Corollary 15. *Let P_n be the USO polytope of Q_n. Let s and t be different USOs and L is the set of edge whose orientations are different in s and t.*

Therefore, (p_s, p_t) is an edge of P_n if L is a single phase of s. Hence, (p_s, p_t) is not an edge if L is the union of multiple phases in s.

PROOF. Suppose L is a single phase of s, $L' \subsetneq L$ and another orientation s' is obtained by flipping all the edges among L' in s. According to Lemma 10, s' is not a USO. Therefore, p_s and p_t is the only two points in the subcube $R(p_s \cap p_t, p_s \cup p_t)$. By Lemma 13, the segment $e = (p_s, p_t)$ is an edge of the polytope P.

Besides, suppose that L is the union of multiple phases, $L = \bigcup_{i=1}^{k} l_i$, where $\forall i \in [k]$, l_i is a single phase of s and $k \geq 2$. Denote s_i as the orientation obtained by flipping the phase l_i in s, thus

$$p_t - p_s = \sum_{i=1}^{k} p_{s_i} - p_s$$

Let $X = \{s, t, s_1, s_2, \cdots, s_k\}$. Notice that $\forall i \in [k]$, s_i is also a USO, thus making p_{s_i} a vertex of P_n. By the above argument, we have (p_s, p_{s_i}) is the edge of P_n. Since $p_t - p_s$ is a conic combination of $p_{s_i} - p_s$, we have (p_s, p_t) is not an edge of $conv(X)$, thus not an edge of P_n. □

REMARK. Notice that in this lemma L is not required to be non-adjacent in s, which is a more general case than Lemma 10.

3.4.4 2-face of USO polytope

Let G_n be the polytope graph of P_n. Once we determine the edges of G_n, we can further aggregate the 2-faces of P_n by the following algorithm 2-FACE DETECTION.

Correctness. For each 2-face f, it can be represented by a 2-dimensional polygon $(p_1, p_2, \cdots, p_3)$, in which $(p_i, p_{i+1}) \in E$. In Line 2-3, we iterate over

Algorithm 1 2-Face Detection

Input: Polytope Graph $G_n = (V, E)$
Output: 2-Faces Set F.

1: $F \leftarrow \varnothing$
2: **for** $u \in V$ **do**
3:     **for** $(u, v) \in E, (u, w) \in E, v \neq w$ **do**
4:         $f \leftarrow \{u, v, w\}$
5:         **for** $p \in V$ **do**
6:             **if** $rank(p - u, v - u, w - u) = 2$ **then**
7:                 $f \leftarrow f \cup \{p\}$
8:             **end if**
9:         **end for**
10:         **if** IsBoundary(f) **then**
11:             $F \leftarrow F \cup \{f\}$
12:         **end if**
13:     **end for**
14: **end for**
15: **return** F

all the possible 2-face by iterating over all the triplets (u, v, w) in which (u, v) and (u, w) are connected in G. Further, we find all the other vertex p such that $p - u \in span\{v - u, w - u\}$, which means p lies in this 2-dimensional subspace, aggregating into the 2-dimensional polygon f. Finally, IsBoundary(f) verifies whether there exists a hyperplane only supports the vertices set $V(f)$, and is implemented by checking the feasibility of the following linear system.

$$w^\top u + b \geq 1, \forall u \notin V(f),$$
$$w^\top u + b = 0, \forall u \in V(f).$$

Efficiency. Let $N = |V|, M = |E|, K = \sum_{u \in V} deg^2(u)$.

The nested loops in Line 2-3 takes in total $O(K)$ iterations. For each possible triplet (u, v, w), it takes $O(N)$ iterations to collect all the other vertices that lie in this spanned subspace. Further, it needs solving a linear program with $n2^{n-1}+1$ variables and N constrains to check whether its exactly supporting the polygon f. Since $n2^n \in o(N)$, the time complexity to solve this linear program is $O(N^\omega)$, where ω is the exponent of matrix multiplication with $\omega \approx 2.38$. Therefore, the overall runtime complexity is $O(N^\omega K + NK) = O(N^\omega K)$.

Acceleration. We accelerate the 2-Face Detection by efficiently computing all the possible 2-faces f, and such improvement is based on the following facts.

Fact 16. *Let P be a 0/1-polytope. For each 2-face f of P, f includes at most 4 vertices of P.*

Proof. Prove this by contradiction. Suppose there exists a 2-face f containing at least 5 vertices, $V(f) = (a, b, c, d, e)$. Denote $U = span\{b-a, c-a, d-a, e-a\}$, and we will show that $dim(U) \geq 3$.

W.L.O.G., we can suppose that $a = \mathbf{0}$. Otherwise, we could apply some linear transformation $T : \{0,1\}^d \to \{0,1\}^d$ to P_n such that $T(a) = \mathbf{0}$ and the $dim(U)$ remains unchanged. Thus, $U = span\{b, c, d, e\}$. Since b, c, d, e are distinct vertices and are not parallel to each other, $dim(U) \geq 2$. Suppose that $dim(U) = 2$ and $\{b, c\}$ is a basis of U.

Consider the following linear indeterminate equation.

$$bx + cy = t, t \in \{0,1\}^d.$$

Since b and c are distinct, there exists i such that $b_i + c_i = 1$. Suppose that $b_i = 1$ and $c_i = 0$. Since $b_i x + c_i y \in \{0,1\}$, we have $x \in \{0,1\}$. Therefore, $(x, y) \in \{(0,0), (0,1), (1,0)\}$ are valid solutions and $(x, y) = (1,1)$ is valid if and only if $b + c \in \{0,1\}^d$. Thus, at most 3 nonzero solutions can be achieved, leading to the contradiction. □

This fact can be generalized to the following lemma.

Lemma 17. *Let P be a 0/1 polytope. For each k-face f of P, f includes at most 2^k vertices.*

Proof Sketch. This can be proved directly by apply induction on the above fact 16. □

Fact 18. *Let P be a 0/1 polytope. For each 2-face f of P, if a 2-face f includes 4 vertices of P, f is a rectangle.*

Proof. According to Fact 14, if a 2-face f includes 4 vertices, it can be formulated as $f = (t, t+a, t+b, t+a+b)$. Notice that $f \subseteq \{0,1\}^d$, we have $\forall i, a_i b_i = 0$ and $a^\top b = 0$. Therefore, f is indeed a rectangle. □

Therefore, for each triplet (u, v, w), the only possible co-planar vertex is $v+w-u$. Having utilized this, we could improve the efficiency of the 2-Face Detection.

Remark. Asymptotically, this acceleration does not improve the complexity. However, it help us to get rid of $O(NK)$ times co-planar check, which is actually useful in practice.

3.5 Isometry

In this section we will discuss the isometry between different USOs, and the isometry on the USO polytope itself. This is also an important reason why we need to regard the set of USOs as a polytope instead of merely on graph structure.

3.5.1 Isomorphic USO

Definition 15. *Two USO s and s' on the hypercube Q^n are called isomorphic to each other if and only if there exist a mapping $f : V(Q_n) \to V(Q_n)$ such that $\forall (u, v) \in E(Q_n)$,*

$$(f(u), f(v)) \in E(Q_n),$$
$$I_s(u, v) = I_{s'}(f(u), f(v)).$$

Briefly, we can say (s, s') admits the isomorphism mapping f, and they are in the same isomorphic class, which means they are identical to each other.

Similarly, we can say s admit the automorphism mapping f if $\forall (u, v) \in E(Q_n)$,

$$(f(u), f(v)) \in E(Q_n),$$
$$I_s(u, v) = I_s(f(u), f(v)).$$

Definition 16. *Let f mapping on $2^{[n]}$, $f : 2^{[n]} \to 2^{[n]}$.*
An identical mapping f is that $f(u) = u$.
A reflection f characterized by $r \in \{0, 1\}^n$ is that $f(u) = u \oplus r$.
A rotation f characterized by $\sigma \in \mathbf{S_n}$ is that $f(u)_{\sigma(i)} = u_i$, where $\mathbf{S_n}$ is the group of all the permutations on $[n]$.

To characterize the isomorphism of the hypercube, we need some other auxiliary lemmas at first.

Lemma 19. *Given a fixed vertex $u \in Q_n$ and its neighbour $N(u)$, for any vertex $v \in Q_n$, it can be uniquely characterized by the distance between v and $u \cup N(u)$.*

In other words, denote $T(u) = u \cup N(u) = \{u_0, u_1, \cdots, u_n\}$, the function $\Gamma : \{0, 1\}^n \to [0, n]^{n+1}$ is injective, where

$$\Gamma(v)_i = d_H(v, u_i), \forall i \in [0, n].$$

Proof. W.L.O.G., suppose $u = \mathbf{0}$. Notice that for any $w \in N(u)$, we have

$$|d_H(u, v) - d_H(w, v)| = 1.$$

Suppose $w_\lambda = 1$. If $d_H(u, v) < d_H(w, v)$, we have $v_\lambda = u_\lambda = 0$. Otherwise, we have $v_\lambda = w_\lambda = 1$. Therefore, for any $\lambda \in [n]$, v_λ is determined its distance from u and $w = \{\lambda\}$, thus making Γ injective. □

Corollary 20. *For any automorphism mapping f of the hypercube Q_n and a fixed vertex $u \in Q_n$, f is uniquely determined by the mapping of u and its neighbour $N(u)$.*

PROOF. Notice that for any (u, v), we have $d_H(u, v) = d_H(f(u), f(v))$. According to Lemma 19, v is uniquely determined by $\Gamma(v)$. Since $\Gamma(v) = \Gamma(f(v))$, $f(v)$ is also uniquely determined. Hence, the automorphism mapping f itself is unique as well. □

Lemma 21. *For any isomorphism mapping f between USOs, it must be composed of a rotation g and a reflection h such that $f = g \circ h$.*

PROOF. Since f is also an automorphism mapping of the hypercube Q_n. It is suffice to prove that despite of the orientation, if the hypercube Q_n admits a automorphism f, f can be decomposed as $f = g \circ h$.

According to 20, suppose that $f(z) = \mathbf{0}$, then f can be decomposed into a reflection $h(u) = u \oplus z$ which is mapping u to $\mathbf{0}$ and a rotation g which is mapping $N(u)$ to neighbour of $\mathbf{0}$. Hence, the automorphism f that agree on this mapping is unique. □

REMARK. As is a direct implication from Lemma 21, we can see that there are $2^n n!$ types of isomorphism on the hypercube Q_n.

3.5.2 Isomorphism Classes

Denote the set of all USOs of Q_n as U and the group of all possible isomorphism mapping on Q_n as F_n respectively. For $s, s' \in U$, they are in the same isomorphic class under F_n if there exists $f \in F_n$ such that $f(s) = s'$. Denote U/F_n as the set of isomorphism classes of U under F_n. According to the Burnside's Lemma [5],

$$|U/F_n| = \frac{1}{|F_n|} \sum_{f \in F} \phi(f),$$

where $\phi(f) = |\{s | f(s) = s, s \in U\}|$, which is the number of fixed points under isomorphism mapping f.

Regard to this, it could better our understanding of the structure of isomorphism classes if we could estimate the number of fixed points that admits a specific automorphism f.

Lemma 22. *Let F_n be the group of all possible isomorphism mapping on Q_n. For any $f \in F_n$ and its decomposition $f = g \circ h$, $h(u) = u \oplus r$ is a reflection and $g(u)_{\sigma(i)} = u_i$ is a rotation, where $\sigma \in \mathbf{S_n}$.*

Hence, we can further decompose the permutation σ into disjoint cycles C such that $\forall c_i$ in C, $c_i = (x_{i,1}, x_{i,2}, \cdots, x_{i,k_i})$ and $\sigma(x_{i,j}) = x_{i,j \mod k_i+1}$.

Denote $\kappa(c_i) = \{k | k \in c_i\}$ and $\tau = \{k | r_k = 1\}$. Then, $\phi(f) \neq 0$ if for any $c_i \in C$, $|\kappa(c_i) \cap \tau|$ is even.

Proof. Generally, we prove this by finding a uniform USO that admits such f.

In a uniform USO s, for any λ-edge e, we have

$$I_s(e) = I_{s,\lambda}, \lambda \in [n],$$

and the uniform USO s can be characterize by the orientation indicator $I_s = (I_{s,1}, I_{s,2}, \cdots, I_{s,n})$. Denote s' as the orientation obtained by operating transformation f on s.

Apart from the reflection h, let us only consider the permutation $g(u)_{\sigma(i)} = u_i$ at first. For any λ-edge (u, v), we have

$$u \oplus v = \lambda,$$
$$g(u) \oplus g(v) = \sigma(\lambda),$$

which shows that g is mapping each λ-edge in s to a $\sigma(\lambda)$-edge in s' and we have $I_{s,\lambda} = I_{s',\sigma(\lambda)}$.

Next, we take the reflection h into consideration. For any λ-edge (u, v) with $u \oplus v = \lambda$, we have

$$g(h(u))) \oplus g(h(v)) = g(u) \oplus g(r) \oplus g(v) \oplus g(r) = \sigma(\lambda),$$

where $f = g \circ h$ is also mapping λ-edges in s to a $\sigma(\lambda)$-edges in s'.

Hence, let $u \subseteq v$, $f(u) \subseteq f(v)$ if and only if $\lambda \notin r$. Therefore,

$$I_{s',\sigma(\lambda)} = \begin{cases} I_{s,\lambda}, & \lambda \notin r, \\ 1 - I_{s,\lambda}, & \lambda \in r. \end{cases}$$

Since s admit the automorphism f, we have $I_s = I_{s'}$. Hence, since each cycle c is disjoint so that we can consider them independently since they are operated on edges of different directions, which is independent from each other. Accordingly, we can assume that σ is a cyclic rotation with length n. It is clear that as long as $|r|$ is even, the above linear system has feasible solution. □

3.5.3 Isomorphic Polytope

Motivation A good example to see why we need seek USO polytope for its combinatorial meanings is as following:

Let s_1 be a USO which only differ from the uniform USO with one edge's orientation incident to its original source. Let s_2 be a USO obtained by flipping all the edges in s_1.

Notice that for any USO s, and the USO s' obtained by flipping all its edges, we have

$$I_s(e) + I_{s'}(e) = 1,$$
$$p_s + p_{s'} = \mathbf{1},$$

which indicating that the USO polytope is central symmetric around the point $p_c = (1/2, 1/2, \cdots, 1/2)$. Therefore, it is clear that the USO polytope should look the same in the point of view at either s or s'.

However, it is clear that s_1 and s_2 are not isomorphic to each other because s_1 differs from a uniform USO by an edge incident to the unique source but s_2 differs by an edge incident to the unique sink, which means that geometric isometry does not always imply graph isometry.

To discuss the geometry isometry of the USO polytope, we need at first properly define it.

Definition 17. *An isometry in the Euclidean space R^d is a distance preserving transformation $f : R^d \to R^d$ such that $\forall x, y$, $\|x - y\|_2 = \|f(x) - f(y)\|_2$, and the group of such isometry is denoted as $\mathbf{SE_d}$.*

The image of a polytope P under then isometry transformation is denoted as $f(P)$, where

$$f(P) = \{f(x)|x \in P\}.$$

For any d-dimensional polytope P and Q, P is isomorphic to Q is there exists $f \in \mathbf{SE_d}$ such that $Q = f(P)$ and $P = f^{-1}(Q)$. Specifically, P admits a automorphism f on itself if $P = f(P)$.

Lemma 23. $\mathbf{SE_d}$ *is composed of any finite composition of translations, rotations, and reflections in R^d.*

Specifically, a d-dimensional Euclidean isometry f is called

- translation, if $f(u) = u + c, c \in R^d$.

- rotation, if $f(u) = Au$, where A is a orthogonal matrix in $R^{d\times d}$.

- reflection, if $f(u) = u - 2\frac{w^\top u+b}{w^\top w}w$, where $H = w^\top x + b = 0$ is the hyperplane that characterizes this reflection.

PROOF. See chapter 1.2 rigid transformation in [8].

Theorem 24. *Let P and Q be d-dimensional polytopes and $X = V(P), Y = V(Q)$ is the vertex set of them respectively. Then, for any $f \in \mathbf{SE_d}$, $f(P) = Q$ if and only if $f(X) = Y$.*

PROOF. $\Rightarrow$: Suppose that $f(P) = Q$. First we argue that $x \in X \Leftrightarrow f(x) \in Y$.

Suppose x is the vertex of P, there exists a supporting hyperplane H of P such that $H \cap P = \{x\}$. By Lemma 24, $f(H)$ is the supporting hyperplane of $f(P)$ and $f(H) \cap f(P) = \{f(x)\}$, thus making $f(x)$ a vertex of the image Q and $f(x) \in Y$.

Suppose $f(x) \in Y$, the similar argument also stands vice versa, as $f^{-1} \in \mathbf{SE_d}$ and we have $X = f^{-1}(Y), x = f^{-1}(f(x)) \in X$, and this concludes the proof of the sufficiency.

$\Leftarrow$: Suppose that $f(X) = Y$. We need to argue that $x \in P \Leftrightarrow f(x) \in Q$.

By Lemma 23, it is clear that for $f \in \mathbf{SE_d}, f(x) = y$, each coordinate y_i is a nonhomogeneous linear combination of x_i, such that

$$y_i = B_i + \sum_{j=1}^{d} A_{i,j}x_i,$$

where $A \in R^{d\times d}, B \in R^d$. Accordingly, we can extend f to another isometry g which is embedded on a hyperplane of R^{d+1} such that $\forall x \in R^d$,

$$h(x) = \begin{bmatrix} x \\ 1 \end{bmatrix},$$

$$g(h(x)) = \begin{bmatrix} A & B \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ 1 \end{bmatrix} = \begin{bmatrix} f(x) \\ 1 \end{bmatrix} = h(f(x)).$$

In other words, g is homogeneous linear transformation characterized by the matrix $\Gamma = \begin{bmatrix} A & B \\ 0 & 1 \end{bmatrix}$, such that $g(x) = \Gamma x$. Hence, denote $M(P) \in R^{d\times n}$ as the matrix whose columns are vertices of a d-dimensional polytope P, in other words, the members of $V(P)$.

Suppose that $x \in P$, it is a convex combination of X, which means that there exist $\Lambda = (\lambda_1, \lambda_2, \cdots, \lambda_n)$, $\lambda_i \geq 0$ and $\sum_{i=1}^{n} \lambda_i = 1$, such that $x = M(P)\Lambda$. Therefore,

$$g(h(x)) = \underbrace{\begin{bmatrix} A & B \\ 0 & 1 \end{bmatrix}}_{\Gamma} \underbrace{\begin{bmatrix} X_1 & \cdots & X_n \\ 1 & \cdots & 1 \end{bmatrix}}_{h(M(P))} \underbrace{\begin{bmatrix} \lambda_1 \\ \cdots \\ \lambda_n \end{bmatrix}}_{\Lambda} = h(f(x)).$$

Since $f(X) = Y$, we have

$$\underbrace{\begin{bmatrix} A & B \\ 0 & 1 \end{bmatrix}}_{\Gamma} \underbrace{\begin{bmatrix} X_1 & \cdots & X_n \\ 1 & \cdots & 1 \end{bmatrix}}_{h(M(P))} = \underbrace{\begin{bmatrix} Y_1 & \cdots & Y_n \\ 1 & \cdots & 1 \end{bmatrix}}_{h(M(Q))},$$

$$f(X_i) = Y_i.$$

Therefore, $g(h(x)) = h(M(Q))\Lambda$. For any $x \in P$, $g(h(x)) = h(f(x))$ is also a convex combination of $h(M(Q))$, indicating $h(f(x)) \in h(Q)$, thus $f(x) \in Q$.

Vice versa, suppose $f(x) \in Q$, the similar argument also stands. Take $f^{-1} \in$ $\mathbf{SE_d}$ and $P = f^{-1}(Q), x = f^{-1}(f(x)) \in P$, thus proving the necessity. $\square$

This theorem provides us a convex len to characterized the isomorphism of polytopes. Instead of considering the whole polytope, it is enough to only focus on the bijection between vertices of the polytope. Nevertheless, the number of such bijection grows exponentially with regard to the number of vertices in P. Therefore, we need further refine the scope of the isomorphism on the USO polytope.

For further analysis, two basic but important facts are needed.

Fact 25. *Let P_n be the USO polytope of Q_n and s be a uniform USO. Let t_i be the USO obtained by flipping the i-th edge in s. Let G be the polytope graph of P_n and $N(u)$ is the neighbour of u in G. Therefore, we have*

$$N(p_s) = \{p_{t_i} | i \in [m], m = n2^{n-1}\}.$$

Proof. First we need to argue that each t_i is indeed a USO. Notice that for a uniform USO s and its outmap S, we have

$$S(u) = u \oplus z,$$

where z is the unique sink of s in Q_n. Therefore, for two λ-edges e_1, e_2 and $u \in e_1, v \in e_2$, we have

$$(u \oplus v) \cap (S(u) \oplus S(v)) = (u \oplus v) \cap (u \oplus z \oplus v \oplus z) = u \oplus v.$$

Notice that $u \oplus v = \{\lambda\}$ only if u, v belong to the same λ-edge. Therefore, for any two λ-edges e_1, e_2, they are not in direct phase to each. Thus, for any edge e_i in s, the phase of it is $\{e_i\}$, which means only flipping itself will lead to another USO t_i.

Next we need to argue that $N(p_s) = \{p_{t_i}\}$. For any USO t other than s, denote L as the set of edges which has different orientations in s and t. Notice that s is a uniform USO and no two edges are in the same phase. Therefore, L is always a union of single or multiple phases. By Corollary 17, (p_s, p_t) is the edge of P_n if and only if $|L| = 1$, indicating that $N(p_s) = \{p_{t_i} | i \in [m], m = n2^{n-1}\}$. □

Remark. Notice that $U = \{p_{t_i} - p_s | i \in [m]\}$ is a orthogonal basis of the space R^m, we have $dim(P_n) = n2^{n-1}$ which is full ranked.

Corollary 26. *Let P_n be the USO polytope of Q_n and s be a uniform USO. Let G be the polytope graph of P_n and $N(u)$ is the neighbour of u in G.*

Suppose that P_n admit an automorphism $f \in \mathbf{SE_m}, m = n2^{n-1}$, then for any USO t of Q_n, $f(p_t)$ can be uniquely determined by the $f(p_s)$ and $f(N(p_s))$.

Proof. For simplicity, let $t_0 = s$ and t_i be the orientation which differs from t_0 by the orientation of the i-th edge.

Let $U = \left[p_{t_0} \ldots p_{t_m}\right]$. Hence, notice that $\{p_{t_i} - p_{t_0} | i \in [m]\}$ is a orthogonal basis of the space $\{0,1\}^m$ and $p_{t_i} \in \{0,1\}^m$. Therefore, for any $y \in \{0,1\}^m$, y belongs to the affine hull of the columns of U. Therefore, there exists $\lambda \in R^{m+1}$ with $\sum_{i=0}^{m} \lambda_i = 1$ such that $y = U\lambda$.

by Lemma 23, $\forall f \in \mathbf{SE_m}$, we have $f(x) = w^\top x + b$, where $w, b \in R^m$. Therefore,

$$\begin{aligned}
f(y) &= w^\top U\lambda + b \\
&= b + \sum_{i=0}^{m} \lambda_i w^\top p_{t_i} \\
&= b + \sum_{i=0}^{m} \lambda_i (f(p_{t_i}) - b) \\
&= \sum_{i=0}^{m} \lambda_i f(p_{t_i}),
\end{aligned}$$

indicating that $f(p_t)$ is characterized by the mapping of p_s and its neighbour $N(p_s)$. □

When it comes to the relationship between hypercube isomorphism and USO polytope isomorphism, here comes the observation.

Fact 27. *Let F_n be the group of isomorphism on the hypercube Q_n and K_n be the group of automorphism on the USO polytope P_n, where $F_n \leq \mathbf{SE_n}$ and $K_n \leq \mathbf{SE_m}, m = n2^{n-1}$. Then, for each $f \in F_n$, it induces a unique automorphism k such that for each USO s and s' obtained by transforming s under f, we have $k(p_s) = p_{s'}$.*

PROOF. Let k be the automorphism in K_n induced by f, and $idx(e)$ be the index of the edge e fixed by the total order in section 3.1. By lemma 23 and Corollary 26, $k = g \circ h$, where g is a permutation and h is a reflection.

For $e_1 = (u_1, v_1), e_2 = (u_2, v_2) \in E(Q_n)$, we denote $f(e_1) = e_2$ if $f(\{u_1, v_1\}) = \{u_2, v_2\}$. Respectively, we construct as g and h as follows. For $f(e_1) = e_2$, let

$$\sigma(idx(e_1)) = idx(e_2),$$
$$g(u)_{\sigma(i)} = i.$$

Hence, for any $f(e_1) = e_2$, let

$$[idx(e_1) \in r] = \begin{cases} 0, & f(u_1) \subseteq f(v_1), \\ 1, & f(v_1) \subseteq f(u_1). \end{cases}$$
$$h(u) = u \oplus r.$$

For orientation s and s' obtained by operating isomorphism f on s, it is clear that $k(p_s) = p_{s'}$. Therefore, k is a bijection on $V(P_n)$ and thus an automorphism of P_n which is induced by f. □

We conclude this section by the following beautiful theorem.

Theorem 28. *Let K_n be the group of automorphism of the USO polytope P_n, then $\forall k \in \mathbf{SE_m}, m = n2^{n-1}$, $k \in K_n$ **if and only if** $k = f \circ h$, where h is a reflection induced by $A \subseteq [n]$ and f is a permutation on $[m]$ induced by some $g \in F_n$.*

INTUITION. For $k \in K_n$, $k(p_s)$ is actually perform some isomorphism $f \in F_n$ on s first, then flipping edges in certain directions.

PROOF. Let $k(p_s) = \mathbf{0}$ and s is a uniform USO, then k can be characterized on the reflection $h(u) = u \oplus p_s$ and the permutation f on the neighbours of p_s, and $k = f \circ h$.

Hence, for any uniform USO s, denote $s(L)$ as the orientation obtained by flipping edges in L from s. Therefore, $\forall e \in E(Q_n)$, we have $s(\{e\})$ is another USO and $\forall e_1, e_2 \in E(Q_n)$, $s(\{e_1, e_2\})$ is another USO if and only if e_1 and e_2 are not adjacent.

Let f be an bijection of $E(Q_n)$, and $t = s(\{e_1, e_2\})$, then

$$k(p_s) = p_{s'},$$
$$k(p_t) = p_{s'(\{f(e_1), f(e_2)\})},$$

where s' is another uniform orientation. Therefore, $f(e_1)$ and $f(e_2)$ are adjacent if and only if e_1 and e_2 are adjacent.

Next we claim that f is actually an automorphism of Q_n, which completes the proof the necessity.

Lemma 29. *Let f be bijection on $E(Q_n)$ such that $\forall e_1, e_2, f(e_1), f(e_2)$ are adjacent if and only if e_1, e_2 are adjacent, then f is actually induced by $g \in F_n : 2^{[n]} \to g^{[n]}$.*

Proof. Construct g explicitly. For each vertex $u \in Q_n$, consider all the edges $e_1, e_2, \cdots, e_n$ incident to vertex u, we have

$$e_1 \cap e_2, \cap \cdots \cap e_n = \{u\}.$$

Notice that $f(e_i)$ are also adjacent to each other pairwise and Q_n is a regular graph of degree n. Therefore, there exists v such that

$$f(e_1) \cap f(e_2), \cap \cdots \cap f(e_n) = \{v\},$$

and let $g(u) = v$ in this case. It is clear that g is uniquely determined by f and for each $g \in F_n$, the induced f also preserve the adjacency of the edges.

To see sufficiency, by fact 26, for each $g \in F_n$, there exists a $f \in K_n$ induced by it, where $f = r \circ t$, where t is a permutation of edges and r is the reflection on certain direction $A \subseteq [n]$.

Compose f with the reflection h, and $k = f \circ h$. By Lemma 2, flipping all the edges in some directions provides us another USO. Therefore,

$$\forall p_s \in P_n, k(p_s) \in P_n.$$

Hence, k is bijective, indicating that $k \in K_n$. $\square$

Remark. As a direct result of theorem 27, we have $|F_n| = n!2^n, |K_n| \leq n!2^{2n}$.

4 Open Questions

We conclude with several open conjectures and potential further discussions, and some are based some interesting observations in our practice.

- For USO s and s' which differs in edge set L, one may conjecture that L always contains a complete phase l_i in s. However, it is not the case but there are only one counter example for $n = 3$. What is the case for higher dimension?
- Lemma 7 provides a necessary condition for USO outmap. If we augment the condition by require each subcube to have such property, what combinatorial structure will we get?
- Corollary 15 actually conclude the case where edges can be decomposed into phases, what about the case where edges are intersecting but not a union of phases?
- Lemma 22 provides a sufficient condition for an automorphism to have non zero fixed points. However, in practice, it is also the necessary condition for $n = 3$. What is the case in higher dimension?
- Lemma 28 consider the relation between K_n and F_n, how is K_n indeed composed of lower dimension isometry?

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