Pseudo Unique Sink Orientations

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Abstract

A unique sink orientation (USO) is an orientation of the \(n\)-dimensional cube graph (\(n\)-cube) such that every face (subcube) has a unique sink. The number of unique sink orientations is \(n^{\Theta(2^n)}\) [13]. If a cube orientation is not a USO, it contains a pseudo unique sink orientation (PUSO): an orientation of some subcube such that every proper face of it has a unique sink, but the subcube itself hasn’t. In this paper, we characterize and count PUSOs of the \(n\)-cube. We show that PUSOs have a much more rigid structure than USOs and that their number is between \(2^{\Omega(2^n - \log n)}\) and \(2^{O(2^n)}\) which is negligible compared to the number of USOs. As tools, we introduce and characterize two new classes of USOs: border USOs (USOs that appear as facets of PUSOs), and odd USOs which are dual to border USOs but easier to understand.

1 Introduction

Unique sink orientations. Since more than 15 years, unique sink orientations (USOs) have been studied as particularly rich and appealing combinatorial abstractions of linear programming (LP) [6] and other related problems [3]. Originally introduced by Stickney and Watson in the context of the P-matrix linear complementarity problem (PLCP) in 1978 [19], USOs have been revived by Szabó and Welzl in 2001, with a more theoretical perspective on their structural and algorithmic properties [20].

The major motivation behind the study of USOs is the open question whether efficient combinatorial algorithms exist to solve PLCP and LP. Such an algorithm is running on a RAM and has runtime bounded by a polynomial in the number of input values (which are considered to be real numbers). In case of LP, the runtime should be polynomial in the number of variables and the number of constraints. For LP, the above open question might be less relevant, since polynomial-time algorithms exist in the Turing machine model since the breakthrough result by
Khachiyan in 1980 [11]. For PLCP, however, no such algorithm is known, so the computational complexity of PLCP remains open.

Many algorithms used in practice for PCLP and LP are combinatorial and in fact simplex-type (or Bard-type, in the LCP literature). This means that they follow a locally improving path of candidate solutions until they either cycle (precautions need to be taken against this), or they get stuck—which in case of PLCP and LP fortunately means that the problem has been solved. The less fortunate facts are that for most known algorithms, the length of the path is exponential in the worst case, and that for no algorithm, a polynomial bound on the path length is known.

USOs allow us to study simplex-type algorithms in a completely abstract setting where cube vertices correspond to candidate solutions, and outgoing edges lead to locally better candidates. Arriving at the unique sink means that the problem has been solved. The requirement that all faces have unique sinks is coming from the applications, but is also critical in the abstract setting itself: without it, there would be no hope for nontrivial algorithmic results [1].

On the one hand, this kind of abstraction makes a hard problem even harder; on the other hand, it sometimes allows us to see what is really going on, after getting rid of the numerical values that hide the actual problem structure. In the latter respect, USOs have been very successful.

For example, in a USO we are not confined to following a path, we can also “jump around”. The fastest known deterministic algorithm for finding the sink in a USO does exactly this [20] and implies the fastest known deterministic combinatorial algorithm for LP if the number of constraints is twice the number of variables [9]. In a well-defined sense, this is the hardest case. Also, RandomFacet, the currently best randomized combinatorial simplex algorithm for LP [10, 14] actually works on acyclic USOs (AUSOs) with the same (subexponential) runtime and a purely combinatorial analysis [5].

The USO abstraction also helps in proving lower bounds for the performance of algorithms. The known (subexponential) lower bounds for RandomFacet and RANDOMEdge—the most natural randomized simplex algorithm—have first been proved on AUSOs [15, 16] and only later on actual linear programs [4]. It is unknown which of the two algorithms is better on actual LPs, but on AUSOs, RANDOMEdge is strictly slower in the worst case [9].

Finally, USOs are intriguing objects from a purely mathematical point of view, and this is the view that we are mostly adopting in in this paper.

**Pseudo unique sink orientations.** If a cube orientation has a unique sink in every face except the cube itself, we call it a pseudo unique sink orientation (PUSO). Every cube orientation that is not a USO contains some PUSO. The
study of PUSOs originates from the master’s thesis of the first author [2] where the PUSO concept was used to obtain improved USO recognition algorithms; see Section 5 below.

One might think that PUSOs have more variety than USOs: instead of exactly one sink in the whole cube, we require any number of sinks not equal to one. But this intuition is wrong: as we show, the number of PUSOs is much smaller than the number of USOs of the same dimension; in particular, only a negligible fraction of all USOs of one dimension lower may appear as facets of PUSOs. These border USOs and the odd USOs— their duals— have a quite interesting structure that may be of independent interest. The discovery of these USO classes and their basic properties, as well as the implied counting results for them and for PUSOs, are the main contributions of the paper.

Overview of the paper. Section 2 formally introduces cubes and orientations, to fix the language. We will define an orientation via its outmap, a function that yields for every vertex its outgoing edges. Section 3 defines USOs and PUSOs and gives some examples in dimensions two and three to illustrate the concepts. In Section 4, we characterize outmaps of PUSOs, by suitably adapting the characterization for USOs due to Szabó and Welzl [20]. Section 5 uses the PUSO characterization to describe a USO recognition algorithm that is faster than the one resulting from the USO characterization of Szabó and Welzl. Section 6 characterizes the USOs that may arise as facets of PUSOs. As these are on the border between USOs and non-USOs, we call them border USOs. Section 7 introduces and characterizes the class of odd USOs that are dual to border USOs under inverting the outmap. Odd USOs are easier to visualize and work with, since in any face of an odd USO we again have an odd USO, a property that fails for border USOs. We also give a procedure that allows us to construct many odd USOs from a canonical one, the Klee-Minty cube. Based on this, Section 8 proves (almost matching) upper and lower bounds for the number of odd USOs in dimension n. Bounds on the number of PUSOs follow from the characterization of border USOs in Section 6. In Section 9 we mention some open problems.

2 Cubes and Orientations

Given finite sets $A \subseteq B$, the cube $C = C^{[A,B]}$ is the graph with vertex set $\text{vert}C = [A, B] := \{V : A \subseteq V \subseteq B\}$ and edges between any two subsets $U, V$ for which $|U \oplus V| = 1$, where $U \oplus V = (U \setminus V) \cup (V \setminus U) = (U \cup V) \setminus (U \cap V)$ is symmetric difference. We sometimes need the following easy fact.

\[(U \oplus V) \cap X = (U \cap X) \oplus (V \cap X).\] (1)
For a cube $C = C^{[A,B]}$, $\dim C := |B \setminus A|$ is its dimension, $\text{carr} C := B \setminus A$ its carrier. A face of $C$ is a subgraph of the form $\mathcal{F} = C^{[I,J]}$, with $A \subseteq I \subseteq J \subseteq B$. If $\dim \mathcal{F} = k$, $\mathcal{F}$ is a $k$-face or $k$-cube. A facet of an $n$-cube $C$ is an $(n-1)$-face of $C$.

If $A = \emptyset$, we abbreviate $C^{[A,B]}$ as $C^B$. The standard $n$-cube is $C^{[n]}$ with $[n] := \{1,2,\ldots,n\}$.

An orientation $\mathcal{O}$ of a graph $G$ is a digraph that contains for every edge $\{U,V\}$ of $G$ exactly one directed edge $(U,V)$ or $(V,U)$. An orientation of a cube $C$ can be specified by its outmap $\phi : \text{vert} C \to 2^{\text{carr} C}$ that returns for every vertex the outgoing coordinates. On every face $\mathcal{F}$ of $C$ (including $C$ itself), the outmap induces the orientation

$$F_{\phi} := (\text{vert} \mathcal{F}, \{(V,V \oplus \{i\}) : V \in \text{vert} \mathcal{F}, i \in \phi(V) \cap \text{carr} \mathcal{F}\}.$$  

In order to actually get a proper orientation of $C$, the outmap must be consistent, meaning that it satisfies $i \in \phi(V) \oplus \phi(V \oplus \{i\})$ for all $V \in \text{vert} C$ and $i \in \text{carr} C$.

Note that the outmap of $F_{\phi}$ is not $\phi$ but $\phi_{\mathcal{F}} : \text{vert} \mathcal{F} \to 2^{\text{carr} \mathcal{F}}$ defined by

$$\phi_{\mathcal{F}}(V) = \phi(V) \cap \text{carr} \mathcal{F}.$$  

(2)

In general, when we talk about a cube orientation $\mathcal{O} = C_{\phi}$, the domain of $\phi$ may be a supercube of $C$ in the given context. This avoids unnecessary indices that we would get in defining $\mathcal{O} = C_{\phi}$ via its “official” outmap $\phi_{C}$. However, sometimes we want to make sure that $\phi$ is actually the outmap of $\mathcal{O}$, and then we explicitly say so.

Figure 1 depicts an outmap and the corresponding 2-cube orientation.

![Outmap](image)

Figure 1: An outmap $\phi$ and the induced 2-cube orientation $C_{\phi}$

### 3 (Pseudo) Unique Sink Orientations

**Definition 1 (USO [20]).** A unique sink orientation (USO) of a cube $C$ is an orientation $C_{\phi}$ such that every face $\mathcal{F}_{\phi}$ has a unique sink. Equivalently, every face $\mathcal{F}_{\phi}$ is a unique sink orientation.
Figure 2 shows the four combinatorially different (pairwise non-isomorphic) orientations of the 2-cube. The eye and the bow are USOs. The twin peak is not a USO since it has two sinks in the whole cube (which is a face of itself). The cycle is not a USO either, since it has no sink in the whole cube. The unique sink conditions for 0- and 1-faces (vertices and edges) are always trivially satisfied.

![Eye, Bow, Twin Peak, Cycle](image)

Figure 2: The 4 combinatorially different orientations of the 2-cube

If an orientation $C_\phi$ is not a USO, there is a smallest face $F_\phi$ that is not a USO. We call the orientation in such a face a pseudo unique sink orientation.

**Definition 2 (PUSO).** A pseudo unique sink orientation (PUSO) of a cube $C$ is an orientation $C_\phi$ that does not have a unique sink, but every proper face $F_\phi \neq C_\phi$ has a unique sink.

The twin peak and the cycle in Figure 2 are the two combinatorially different PUSOs of the 2-cube. The 3-cube has 19 combinatorially different USOs [19], but only two combinatorially different PUSOs, see Figure 3 together with Corollary 13 below.

![3D Cube Diagrams](image)

Figure 3: The two combinatorially different PUSOs of the 3-cube

We let $uso(n)$ and $puso(n)$ denote the number of USOs and PUSOs of the standard $n$-cube. We have $uso(0) = 1$, $uso(1) = 2$ as well as $uso(2) = 12$ (4 eyes and 8 bows). Moreover, $puso(0) = puso(1) = 0$ and $puso(2) = 4$ (2 twin peaks, 2 cycles).

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1The naming goes back to Szabó and Welzl [20].
4 Outmaps of (Pseudo) USOs

Outmaps of USOs have a simple characterization \([20, \text{Lemma 2.3}]\): \(\phi : \text{vert}C \rightarrow 2^{\text{carr}C}\) is the outmap of a USO of \(C\) if and only if

\[(\phi(U) \oplus \phi(V)) \cap (U \oplus V) \neq \emptyset\]  

(3)

holds for all pairs of distinct vertices \(U, V \in \text{vert}C\). This condition means the following: within the face \(C[U \cap V, U \cup V]\) spanned by \(U\) and \(V\), there is a coordinate that is outgoing for exactly one of the two vertices. In particular, any two distinct vertices have different outmap values, so \(\phi\) is injective and hence bijective.

This characterization implicitly makes a more general statement: for every face \(F\), orientation \(F\phi\) is a USO if and only if (3) holds for all pairs of distinct vertices \(U, V \in F\). The reason is that the validity of (3) only depends on the behavior of \(\phi\) within the face spanned by \(U\) and \(V\). Formally, for \(U, V \in F\), (3) is equivalent to the USO-characterizing condition \((\phi_F(U) \oplus \phi_F(V)) \cap (U \oplus V) \neq \emptyset\) for the orientation \(F\phi_F = F\phi\).

**Lemma 3.** Let \(C\) be a cube, \(\phi : \text{vert}C \rightarrow 2^{\text{carr}C}\), \(F\) a face of \(C\). Then \(F\phi\) is a USO if and only if

\[(\phi(U) \oplus \phi(V)) \cap (U \oplus V) \neq \emptyset\]  

holds for all pairs of distinct vertices \(U, V \in \text{vert}F\). In this case, the outmap \(\phi_F\) of \(F\phi\) is bijective.

As a consequence, outmaps of PUSOs can be characterized as follows: (3) holds for all pairs of non-antipodal vertices \(U, V \in \text{vert}C\) (which always span a proper face), but fails for some pair \(U, V = \text{carr}C \setminus U\) of antipodal vertices. As the validity of (3) is invariant under replacing all outmap values \(\phi(V)\) with \(\phi'(V) = \phi(V) \oplus R\) for some fixed \(R \subseteq \text{carr}C\), we immediately obtain that PUSOs (as well as USOs [20, Lemma 2.1]) are closed under flipping coordinates (reversing all edges along some subset of the coordinates).

**Lemma 4.** Let \(C\) be a cube, \(\phi : \text{vert}C \rightarrow 2^{\text{carr}C}\), \(F\) a face of \(C\). Suppose that \(F\phi\) is a PUSO and \(R \subseteq \text{carr}C\). Consider the \(R\)-flipped orientation \(C_{\phi'}\) induced by the outmap

\[\phi'(V) := \phi(V) \oplus R, \quad \forall V \in \text{vert}C.\]

Then \(F_{\phi'}\) is a PUSO as well.

Using this, we can show that in a PUSO, (3) must actually fail on all pairs of antipodal vertices, not just on some pair, and this is the key to the strong structural properties of PUSOs.
Theorem 5 (PUSO characterization). Let $C$ be a cube of dimension at least 2, $\phi : \text{vert} C \to 2^\text{arr} C$, $F$ a face of $C$. Then $F_\phi$ is a PUSO if and only if

(i) condition (3) holds for all $U, V \in \text{vert} F, V \neq U, \text{carr} F \setminus U$ (pairs of distinct, non-antipodal vertices in $F$), and

(ii) condition (3) fails for all $U, V \in \text{vert} F, V = \text{carr} F \setminus U$ (pairs of antipodal vertices in $F$).

Proof. In view of the above discussion, it only remains to show that (ii) holds if $F_\phi$ is a PUSO. Let $U \in \text{vert} F$. Applying Lemma 4 with $R = \phi(U)$ does not affect the validity of (3), so we may assume w.l.o.g. that $\phi(U) = \emptyset$, hence $U$ is a sink in $F_\phi$. For a non-antipodal $W \in \text{vert} F$, (i) implies the existence of some $i \in \phi(W) \cap (U \oplus W) \subseteq \phi(W) \cap \text{carr} F = \phi_F(W)$, hence such a $W$ is not a sink in $F_\phi$. But then $V = \text{carr} F \setminus U$ must be a second sink in $F_\phi$, because PUSO $F_\phi$ does not have a unique sink. This in turn implies that (3) fails for $U, V = \text{carr} F \setminus U$. \qed

Corollary 6. Let $C_\phi$ be a PUSO with outmap $\phi$.

(i) Any two antipodal vertices $U, V = \text{carr} C \setminus U$ have the same outmap value, $\phi(U) = \phi(V)$.

(ii) $C_\phi$ either has no sink, or exactly two sinks.

Proof. For antipodal vertices, $U \oplus V = \text{carr} C$, so $(\phi(U) \oplus \phi(V)) \cap (U \oplus V) = \emptyset$ is equivalent to $\phi(U) = \phi(V)$. In particular, the number of sinks is even but cannot exceed 2, as otherwise, there would be two non-antipodal sinks; the proper face they span would then have more than one sink, a contradiction. \qed

We can use the characterization of Theorem 5 to show that PUSOs exist in every dimension $n \geq 2$.

Lemma 7 (PUSO Existence). Let $n \geq 2$, $C$ the standard $n$-cube and $\pi : [n] \to [n]$ a permutation consisting of a single $n$-cycle. Consider the function $\phi : 2^{[n]} \to 2^{[n]}$ defined by $\phi(V) = \{i \in [n] : |V \cap \{i, \pi(i)\}| = 1\}, \forall V \subseteq [n]$. Then $C_\phi$ is a PUSO.

Proof. According to Theorem 5, we need to show that condition (3) fails for all pairs of antipodal vertices, but that it holds for all pairs of distinct vertices that are not antipodal.

We first consider two antipodal vertices $U$ and $V = [n] \setminus U$ in which case we get $\phi(U) = \phi(V)$, so (3) fails. If $U$ and $V$ are distinct and not antipodal, there is some coordinate in which $U$ and $V$ differ, and some coordinate in which $U$ and $V$
agree. Hence, if we traverse the $n$-cycle $(1, \pi(1), \pi(\pi(1)), \ldots)$, we eventually find two consecutive elements $i, \pi(i)$ such that $U$ and $V$ differ in coordinate $i$ but agree in coordinate $\pi(i)$, meaning that $i \in (\phi(U) \oplus \phi(V)) \cap (U \oplus V)$, so (3) holds.

We conclude this section with another consequence of Theorem 5 showing that PUSOs have a parity.

**Lemma 8.** Let $C_{\phi}$ be a PUSO with outmap $\phi$. Then the outmap values of all vertices have the same parity, that is

$$|\phi(U) \oplus \phi(V)| = 0 \mod 2, \quad \forall U, V \in \text{vert}C.$$

We call the number $|\phi(\emptyset)| \mod 2$ the parity of $C_{\phi}$. By Corollary 6, a PUSO of even parity has two sinks, a PUSO of odd parity has none.

**Proof.** We first show that the outmap value of any two distinct non-antipodal vertices $U$ and $V$ differ in at least two coordinates. Let $V'$ be the antipodal vertex of $V$. As $U$ is neither antipodal to $V$ nor to $V'$, Theorem 5 along with $\phi(V) = \phi(V')$ (Corollary 6) yields

$$(\phi(U) \oplus \phi(V)) \cap (U \oplus V) \neq \emptyset,$$

$$(\phi(U) \oplus \phi(V)) \cap (U \oplus V') \neq \emptyset.$$

Since $U \oplus V$ is disjoint from $U \oplus V'$, $\phi(U) \oplus \phi(V)$ contains at least two coordinates.

Now we can prove the actual statement. Let $I$ be the image of $\phi$, $I := \{\phi(V) : V \in \text{vert}C\} \subseteq C' = C_{\text{car}C}$. We have $|I| \geq 2^{n-1}$, because by Lemma 3, $\phi_{\mathcal{F}}$ is bijective (and hence $\phi$ is injective) on each facet $\mathcal{F}$ of $C$. On the other hand, $I$ forms an independent set in the cube $C'$, as any two distinct outmap values differ in at least two coordinates; The statement follows, since the only independent sets of size at least $2^{n-1}$ in an $n$-cube are formed by all vertices of fixed parity.

\section{Recognizing (Pseudo) USOs}

Before we dive deeper into the structure of PUSOs in the next section, we want to present a simple algorithmic consequence of the PUSO characterization provided by Theorem 5.

Suppose that $C$ is an $n$-cube, and that an outmap $\phi : \text{vert}C \rightarrow 2^{\text{car}C}$ is succinctly given by a Boolean circuit of polynomial size in $n$. Then it is coNP-complete to decide whether $C_{\phi}$ is a USO \cite{7}. coNP-membership is easy: every non-USO has a certificate in the form of two vertices that fail to satisfy (3). Finding two such vertices
vertices is hard, though. For given vertices $U$ and $V$, let us call the computation of $(\phi(U) \oplus \phi(V)) \cap (U \oplus V)$ a \textit{pair evaluation}. Then, the obvious algorithm needs $\Theta(4^n)$ pair evaluations. Using Theorem \ref{thm:fasterUSO}, we can improve on this.

\textbf{Theorem 9 (Faster USO recognition).} \textit{Let $C$ be an $n$-cube, $\phi : \text{vert} C \to 2^{\text{carr} C}$. Using $O(3^n)$ pair evaluations, we can check whether $C \phi$ is a USO.}

\textit{Proof.} For every face $F$ of dimension at least 1 (there are $3^n - 2^n$ of them), we perform a pair evaluation with an arbitrary pair of antipodal vertices $U, V = \text{carr} F \setminus U$. We output that $C \phi$ is a USO if and only if all these pair evaluations succeed (meaning that they return nonempty sets).

We need to argue that this is correct. Indeed, if $C \phi$ is a USO, all pair evaluations succeed by Lemma \ref{lem:paireval}. If $C \phi$ is not a USO, it is either not an orientation (so the pair evaluation in some 1-face fails), or it contains a PUSO $\mathcal{F} \phi$ in which case the pair evaluation in $F$ fails by Theorem \ref{thm:pairevalfails}.

Using the same algorithm, we can also check whether $C \phi$ is a PUSO. Which is the case if and only if the pair evaluation succeeds on every face except $C$ itself.

\section{6 Border Unique Sink Orientations}

Lemma \ref{lem:nofacets} already implies that not every USO can occur as a facet of a PUSO. For example, let us assume that an eye (Figure \ref{fig:eye}) appears as a facet of a 3-dimensional PUSO. Then, Corollary \ref{cor:mirrororientation}(i) completely determines the orientation in the opposite facet: we get a “mirror orientation” in which antipodal vertices have traded outgoing coordinates; see Figure \ref{fig:mirrororientation}.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{mirrororientation.png}
\caption{An eye is not a facet of a PUSO}
\end{figure}

But now, every edge between the two facets connects two vertices with the same outmap parity within their facets, and no matter how we orient the edge, the two vertices will receive different global outmap parities. Hence, the resulting orientation cannot be a PUSO by Lemma \ref{lem:nofacets}. 

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It therefore makes sense to study the class of border USOs, the USOs that appear as facets of PUSOs.

**Definition 10** (Border USO). A border USO is a USO that is a facet of some PUSO.

If the border USO lives on cube \( F = C^{[A,B]} \), the PUSO may live on \( C^{[A,B \cup \{n\}]} \) \((n \notin \text{carr} F\) a new coordinate), or on \( C^{[A \setminus \{n\},B]} \) \((n \in A)\), but these cases lead to combinatorially equivalent situations. We will always think about extending border USOs by adding a new coordinate.

In this section, we characterize border USOs. We already know that antipodal vertices must have outmap values of different parities; a generalization of this yields a sufficient condition: if the outmap values of distinct vertices \( U,V \) agree outside of the face spanned by \( U \) and \( V \), then the two outmap values must have different parities.

**Theorem 11** (Border USO characterization). Let \( F_\psi \) be a USO with outmap \( \psi \). \( F_\psi \) is a border USO if and only if the following condition holds for all pairs of distinct vertices \( U,V \in \text{vert} F \):

\[
\psi(U) \oplus \psi(V) \subseteq U \oplus V \Rightarrow |\psi(U) \oplus \psi(V)| = 1 \mod 2. \quad (4)
\]

A preparatory step will be to generalize the insight gained from the case of the eye above and show that a USO can be extended to a PUSO of one dimension higher in at most two canonical ways—exactly two if the USO is actually border.

**Lemma 12.** Let \( F \) be a facet of \( C \), \( \text{carr} C \setminus \text{carr} F = \{n\} \), and let \( F_\psi \) be a USO with outmap \( \psi \).

(i) There are at most two outmaps \( \phi : \text{vert} C \rightarrow 2^{\text{carr} C} \) such that \( C_\phi \) is a PUSO with \( F_\phi = F_\psi \). Specifically, these are \( \phi_i, i = 0, 1, \) with

\[
\phi_i(V) = \begin{cases} 
\psi(V), & V \in \text{vert} F, \ |\psi(V)| = i \mod 2, \\
\psi(V) \cup \{n\}, & V \in \text{vert} F, \ |\psi(V)| \neq i \mod 2, \\
\phi_i(\text{carr} C \setminus V), & V \notin \text{vert} F.
\end{cases} \quad (5)
\]

(ii) If \( F_\psi \) is a border USO, both \( C_{\phi_0} \) and \( C_{\phi_1} \) are PUSOs.

(iii) If \( C_{\phi_i} \) is a PUSO for some \( i \in \{0,1\} \), then \( C_{\phi_{1-i}} \) is a PUSO as well, and \( F_\psi \) is a border USO.

**Proof.** Only for \( \phi = \phi_i, i = 0, 1 \), we obtain \( F_\phi = F_\psi \) and satisfy the necessary conditions of Corollary \[\text{(pairs of antipodal vertices have the same outmap values}]

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in a PUSO), and of Lemma 8 (all outmap values have the same parity in a PUSO).
Hence, $C_{\phi_0}$ and $C_{\phi_1}$ are the only candidates for PUSOs extending $F_\psi$.
This yields (i). If $F_\psi$ is a border USO, one of the candidates is a PUSO by definition; as
the other one results from it by just flipping coordinate $n$, it is also a PUSO by
Lemma 4. Part (ii) follows. For part (iii), we use that $F_\psi$ is a facet of $C_{\phi_i}$, $i = 0, 1$,
so as before, if one of the latter is a PUSO, then both are, and $F_\psi$ is a border USO
by definition.

**Corollary 13.** There are 2 combinatorially different PUSOs of the 3-cube (depicted in Figure 3).

**Proof.** We have argued above that an eye cannot be extended to a PUSO, so
let us try to extend a bow (the front facet in Figure 3). The figure shows the
two candidates for PUSOs provided by Lemma 12. Both happen to be PUSOs,
so starting from the single combinatorial type of 2-dimensional border USOs, we
arrive at the two combinatorial types of 3-dimensional PUSOs.

Concluding this section, we prove the advertised characterization of border USOs.

**Proof.** [Theorem 11] Let $C$ be a cube with facet $F$, $\text{carr} C \setminus \text{carr} F = \{n\}$. We show
that condition (6) fails for some pair of distinct vertices $U, V \in \text{vert} F$ if and only
if $C_{\phi_0}$ is not a PUSO, with $\phi_0$ as in (5). By Lemma 12, this is equivalent to $F_\psi$
not being a border USO.

Suppose first that there are distinct $U, V \in \text{vert} F$ such that $\psi(U) \oplus \psi(V) \subseteq
U \oplus V$ and $|\psi(U) \oplus \psi(V)| = 0 \mod 2$, meaning that $U$ and $V$ have the same
outmap parity. By definition of $\phi_0$, we then get

$$\psi(U) \oplus \psi(V) = \phi_0(U) \oplus \phi_0(V) = \phi_0(U) \oplus \phi_0(V') \subseteq U \oplus V,$$

where $V' = \text{carr} C \setminus V$ is antipodal to $V$ in $C$. Moreover, as $U \oplus V$ is also antipodal
to $U \oplus V'$, the inclusion $\phi_0(U) \oplus \phi_0(V) = \phi_0(U) \oplus \phi_0(V') \subseteq U \oplus V$ is equivalent to

$$(\phi_0(U) \oplus \phi_0(V')) \cap (U \oplus V') = \emptyset. \quad (6)$$

Since $U, V$ are distinct and non-antipodal (in $C$), $U, V'$ are therefore distinct non-
antipodal vertices that fail to satisfy Theorem 5 (i), so $C_{\phi_0}$ is not a PUSO.

For the other direction, we play the movie backwards. Suppose that $C_{\phi_0}$ is not
a PUSO. As pairs of antipodal vertices comply with Theorem 5 (ii) by definition
of $\phi_0$, there must be distinct and non-antipodal vertices $U, V'$ with the offending
property (6). Moreover, as $\phi_0$ induces USOs on both $F$ (where we have $F_\psi$) and its
opposite facet $F'$ (where we have a mirror image of $F_\psi$), Lemma 3 implies that $U$
and $V'$ cannot both be in $F$, or in $F'$. W.l.o.g. assume that $U \in \text{vert} F, V' \in \text{vert} F'$,
and let $V \in \text{vert}\mathcal{F}$ be antipodal to $V'$. Then, as before, (6) is equivalent to the inclusion $\phi_0(U) \oplus \phi_0(V) = \phi_0(U) \oplus \phi_0(V') \subseteq U \oplus V$. In particular, $\phi_0(U)$ and $\phi_0(V)$ must agree in coordinate $n$ which in turn implies

$$\psi(U) \oplus \psi(V) = \phi_0(U) \oplus \phi_0(V) \subseteq U \oplus V;$$

and since $|\phi_0(U) \oplus \phi_0(V)| = 0 \mod 2$ by definition of $\phi_0$, we have found two distinct vertices $U, V \in \text{vert}\mathcal{F}$ that fail to satisfy (4).

For an example of a 3-dimensional border USO, see Figure 5. In particular, we see that faces of border USOs are not necessarily border USOs: an eye cannot be a 2-dimensional border USO (Figure 4), but it may appear in a facet $\mathcal{F}$ of a 3-dimensional border USO (for example, the bottom facet in Figure 5), since the incident edges along the third coordinate can be chosen such that (4) does not impose any condition on the USO in $\mathcal{F}$.

Figure 5: A border USO with eyes (non-border USOs) in the bottom and the top facet

Let $\text{border}(n)$ denote the number of border USOs of the standard $n$-cube. By Lemma 12,

$$\text{puso}(n) = 2\text{border}(n - 1), \quad n \geq 2. \quad (7)$$

### 7 Odd Unique Sink Orientations

By (7), counting PUSOs boils down to counting border USOs. However, as faces of border USOs are not necessarily border USOs (see the example of Figure 5), it will be easier to work in a dual setting where we get a class of USOs that is closed under taking faces.

**Lemma 14.** Let $\mathcal{C}_\phi$ be a USO of $\mathcal{C} = \mathcal{C}^B$ with outmap $\phi$. Then $\mathcal{C}_{\phi^{-1}}$ is a USO as well, the dual of $\mathcal{C}_\phi$. 

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Proof. We use the USO characterization of Lemma 3. Since $C_\phi$ is a USO, $\phi : 2^B \to 2^B$ is bijective to begin with, so $\phi^{-1}$ exists. Now let $U', V' \in \text{vert} C$, $U' \neq V'$ and define $U := \phi^{-1}(U') \neq \phi^{-1}(V') =: V$. Then we have

$$(\phi^{-1}(U') \oplus \phi^{-1}(V')) \cap (U' \cap V') = (U \oplus V) \cap (\phi(U) \oplus \phi(V)) \neq \emptyset,$$

since $C_\phi$ is a USO. Hence, $C_{\phi^{-1}}$ is a USO as well.

**Definition 15 (Odd USO).** An odd USO is a USO that is dual to a border USO.

Figure 6 shows an example of the duality with the following outmaps:

| $V$  | $\emptyset$ | $\{1\}$ | $\{2\}$ | $\{3\}$ | $\{1,2\}$ | $\{1,3\}$ | $\{2,3\}$ | $\{1,2,3\}$ | $\phi^{-1}(V')$ |
|------|-------------|---------|---------|---------|---------|---------|---------|-----------|-------------|
| $\phi(V)$ | $\emptyset$ | $\{1\}$ | $\{1,2\}$ | $\{2,3\}$ | $\{2\}$ | $\{1,2,3\}$ | $\{1,3\}$ | $\{3\}$ | $V'$         |

Figure 6: The border USO $C_\phi$ of Figure 5 (left) and its dual odd USO $C_{\phi^{-1}}$ (right). The labels denote the vertices.

A characterization of odd USOs now follows from Theorem 11 by swapping the roles of vertices and outmaps; the proof follows the same scheme as the one of Lemma 14 and is omitted.

**Theorem 16 (Odd USO characterization).** Let $C_\phi$ be a USO with outmap $\phi$. $C_\phi$ is an odd USO if and only if the following condition holds for all pairs of distinct vertices $U, V \in \text{vert} C$:

$$U \oplus V \subseteq \phi(U) \oplus \phi(V) \quad \Rightarrow \quad |U \oplus V| = 1 \mod 2.$$ (8)

In words, if the outmap values of two distinct vertices $U, V$ differ in all coordinates within the face spanned by $U$ and $V$, then $U$ and $V$ are of odd Hamming distance. As this property also holds for any two distinct vertices within a face $F$, this implies the following.

---

Hamming distance is defined for two bit vectors, but we can also define it for two sets in the obvious way as the size of their symmetric difference.
Corollary 17. Let $C_\phi$ be an odd USO, $F$ a face of $C$.

(i) $F_\phi$ is an odd USO.

(ii) If $\dim(F) = 2$, $F_\phi$ is a bow.

Indeed, as source and sink of an eye violate (8), all 2-faces of odd USOs are bows. To make the global structure of odd USOs more transparent, we develop an alternative view on them in terms of caps that can be considered as “higher-dimensional bows”.

Definition 18 (Cap). Let $C_\phi$ be an orientation with bijective outmap $\phi$. For $W \in \text{vert} C$, let $\overline{W} \in \text{vert} C$ be the unique complementary vertex, the one whose outmap value is antipodal to $\phi(W)$; formally, $\phi(W) \oplus \phi(\overline{W}) = \text{carr} C$. $C_\phi$ is called a cap if

$$|W \oplus \overline{W}| = 1 \mod 2, \quad \forall W \in \text{vert} C.$$

Figure 7 illustrates this notion on three examples.

Figure 7: A 3-dimensional cap: complementary vertices (vertices that differ in all outgoing coordinates) have odd Hamming distance (left); the eye is not a cap (middle); the bow is a cap (right).

Lemma 19. Let $C_\phi$ be an orientation with outmap $\phi$. $C_\phi$ is an odd USO if and only if all its faces are caps.

Proof. If all faces are caps, their outmaps are bijective, meaning that all faces have unique sinks. So $C_\phi$ is a USO. It is odd, since the characterizing property (8) follows for all distinct $U, V$ via the cap spanned by $U$ and $V$.

Now suppose that $C_\phi$ is an odd USO. Then every face $F$ has a bijective outmap to begin with, by Lemma 3 to show that $F$ is a cap, consider any two complementary vertices $W, \overline{W}$ in $F$. As $W$ and $\overline{W}$ are in particular complementary in the face that they span, they have odd Hamming distance by (8).
There is a “canonical” odd USO of the standard \( n \)-cube in which the Hamming distances of complementary vertices are not only odd, but in fact always equal to 1. This orientation is known as the Klee-Minty cube, as it captures the combinatorial structure of the linear program that Klee and Minty used in 1972 to show for the first time that the simplex algorithm may take exponential time \[12\].

The \( n \)-dimensional Klee-Minty cube can be defined inductively: \( \text{KM}^{[n]} \) is obtained from \( \text{KM}^{[n-1]} \) by embedding an \([n-1]\)-flipped copy of \( \text{KM}^{[n-1]} \) into the opposite facet \( C^{[\{n\}]} \), with all connecting edges oriented towards \( C^{[n-1]} \); the resulting USO contains a directed Hamiltonian path; see Figure 8. As a direct consequence of the construction, \( \text{KM}^{[n]} \) is a cap: complementary vertices are neighbors along coordinate \( n \). Moreover, it is easy to see that each \( k \)-face is combinatorially equivalent to \( \text{KM}^{[k]} \), hence all faces are caps, so \( \text{KM}^{[n]} \) is an odd USO.

![Figure 8: The Klee-Minty cubes KM[1], KM[2], KM[3] (with pairs of complementary vertices and directed Hamiltonian path)](image)

Next, we do this more formally, as we will need the Klee-Minty cube as a starting point for generating many odd USOs.

**Lemma 20.** Consider the standard \( n \)-cube \( C \) and the outmap \( \phi: 2^{[n]} \rightarrow 2^{[n]} \) with

\[
\phi(V) = \{ j \in [n] : |V \cap \{ j, j + 1, \ldots, n \}| = 1 \mod 2 \}, \quad \forall V \subseteq [n].
\]

Then \( \text{KM}^{[n]} := C_\phi \) is an odd USO that satisfies

\[
\phi(W) \oplus \phi(W \oplus \{ i \}) = [i], \quad \forall i \in [n].
\] (9)

for each vertex \( W \).

In particular, for all \( i \) and \( W \in C^{[i-1]} \), \( W \) and \( W \cup \{ i \} \) are complementary in \( C^{[i]} \), so we recover the above inductive view of the Klee-Minty cube.

**Proof.** We first show that

\[
\phi(U) \oplus \phi(V) = \phi(U \oplus V), \quad \forall U, V \subseteq [n].
\] (10)
Indeed, $j \in \phi(U) \oplus \phi(V)$ is equivalent to $U \cap \{j, j+1, \ldots, n\}$ and $V \cap \{j, j+1, \ldots, n\}$ having different parities, which by (1) is equivalent to $(U \oplus V) \cap \{j, j+1, \ldots, n\}$ having odd parity, meaning that $j \in \phi(U \oplus V)$.

Since $\phi(U) \oplus \phi(V) = \phi(U \oplus V)$ contains the largest element of $U \oplus V$, (3) holds for all pairs of distinct vertices, so $C_\phi$ is a USO. Condition (9) follows from

$$
\phi(W) \oplus \phi(W \oplus \{i\}) = \phi([i]) = [i].
$$

To show that $C_\phi$ is odd, we verify condition (8) of Theorem 16. Suppose that $U \oplus V \subseteq \phi(U) \oplus \phi(V) = \phi(U \oplus V)$ for two distinct vertices. Since $\phi(U \oplus V)$ does not contain the second-largest element of $U \oplus V$, the former inclusion can only hold if there is no such second-largest element, i.e. $U$ and $V$ have (odd) Hamming distance 1.

The Klee-Minty cube has a quite special property: complementing any vertex (reversing all its incident edges) yields another odd USO. Even more is true: any set of vertices with disjoint neighborhoods can be complemented simultaneously. Thus, if we select a set of $N$ vertices with pairwise Hamming distance at least 3, we get $2^N$ different odd USOs. We will use this in the next section to get a lower bound on the number of odd USOs. The following lemma is our main workhorse.

**Lemma 21.** Let $C_\phi$ be an odd USO of the standard $n$-cube with outmap $\phi$, $W \in \text{vert} C$ a vertex satisfying condition (9): $\phi(W) \oplus \phi(W \oplus \{i\}) = [i], \ \forall i \in [n]$.

Let $C_{\phi'}$ be the orientation resulting from complementing (reversing all edges incident to) $W$. Formally,

$$
\phi'(W) = \phi(W) \oplus [n], \\
\phi'(W \oplus \{i\}) = \phi(W \oplus \{i\}) \oplus \{i\}, \ i = 1, \ldots, n,
$$

and $\phi'(V) = \phi(V)$ for all other vertices. Then $C_{\phi'}$ is an odd USO as well.

**Proof.** We first show that every face $F_{\phi'}$ has a unique sink, so that $\phi'$ is a USO. If $W \not\in \text{vert} F$, then $F_{\phi'} = F_{\phi}$, so there is nothing to show. If $W \in \text{vert} F$, let $\text{carr} F = \{i_1, i_2, \ldots, i_k\}, i_1 < i_2 < \cdots < i_k$. Using (1), condition (9) yields

$$
\phi_F(W) \oplus \phi_F(W \oplus \{i_t\}) = \{i_1, i_2, \ldots, i_t\}, \ \forall t \in [k]
$$

and further

$$
\phi_F(W \oplus \{i_s\} \oplus \phi_F(W \oplus \{i_t\}) = \{i_{s+1}, i_{s+2}, \ldots, i_t\}, \ \forall s, t \in [k], s < t.
$$

In general, the operation of complementing a vertex will destroy the USO property.
In particular, $W$ is complementary to $W \oplus \{i_k\}$ in $F$, but this is the only complementary pair among the $k+1$ vertices in $F$ that are affected by complementing $W$. From (11), it similarly follows that
\[
\phi'_F(W) = \phi_F(W) \oplus \{i_1, i_2, \ldots, i_k\} \quad (12),
\]
\[
\phi'_F(W \oplus \{i_1\}) = \phi_F(W \oplus \{i_1\}) \oplus \{i_1\} \quad (12),
\]
\[
\phi'_F(W \oplus \{i_t\}) = \phi_F(W \oplus \{i_t\}) \oplus \{i_t\} \quad (13),
\]
for $t = 2, \ldots, k$. This means that the $k+1$ affected vertices just permute their outmap values under $\phi_F \rightarrow \phi'_F$. This does not change the number of sinks, so $F_{\phi'}$ has a unique sink as well.

It remains to show that $F_{\phi'}$ is a cap, so $C_{\phi'}$ is an odd USO by Lemma [19]. Since $F_{\phi}$ is a cap, it suffices to show that complementary vertices keep odd Hamming distance under $\phi_F \rightarrow \phi'_F$. This can also be seen from (14): for $t = 2, \ldots, k$, the vertex of outmap value $\phi_F(W \oplus \{i_t-1\})$ moves by Hamming distance 2, namely from $W \oplus \{i_t-1\}$ (under $\phi_F$) to $W \oplus \{i_t\}$ (under $\phi'_F$). Hence it still has odd Hamming distance to its unaffected complementary vertex. The two complementary vertices of outmap values $\phi_F(W)$ and $\phi_F(W \oplus \{i_k\})$ move by Hamming distance 1 each. Vertices of other outmap values are unaffected.

As an example, if we complement the vertex $Y$ in the Klee-Minty cube of Figure 8, we obtain the odd USO in Figure 7 (left); see Figure 9. Vertices $X$ and $Z$ have moved by Hamming distance 2, while $Y$ and $Y'$ have moved by Hamming distance 1 each. If we subsequently also complement $W$ (whose neighborhood was unaffected, so Lemma [21] still applies), we obtain another odd USO (actually, a rotated Klee-Minty cube).

![Figure 9: Complementing the two vertices $Y, W$ in succession, starting from the Klee-Minty cube (left)](image)

Let odd($n$) denote the number of odd USOs of the standard $n$-cube. By Definition [15] we get
\[
\text{odd}(n) = \text{border}(n), \quad \forall n \geq 0,
\]
(15)
as duality (Lemma 14) is a bijection on the set of all USOs.

8 Counting PUSOs and odd USOs

With characterizations of USOs, PUSOs, border USOs, and odd USOs available, one can explicitly enumerate these objects for small dimensions. Here are the results up to dimension 5 (the USO column is due to Schurr [17, Chapter 6]). We remark that most numbers (in particular, the larger ones) have not independently been verified.

| $n$ | $\text{uso}(n)$ | $\text{puso}(n) = 2\text{border}(n - 1)$ | $\text{border}(n) = \text{odd}(n)$ |
|-----|-----------------|----------------------------------------|----------------------------------|
| 0   | 1               | 0                                      | 1                                |
| 1   | 2               | 0                                      | 2                                |
| 2   | 12              | 4                                      | 8                                |
| 3   | 744             | 16                                     | 112                              |
| 4   | $5'541'744$     | 224                                    | 12'928                           |
| 5   | $638'560'878'292'512$ | 25'856                                | 44'075'264                      |

Table 1: The number of USOs, PUSOs and border / odd USOs of the standard $n$-cube, obtained through computer enumeration

The number of PUSOs appears to be very small, compared to the total number of USOs of the same dimension. In this section, we will show the following asymptotic results that confirms this impression.

**Theorem 22** (Counting PUSOs). Let $\text{puso}(n)$ denote the number of PUSOs of the standard $n$-cube.

(i) For $n \geq 2$, $\text{puso}(n) \leq 2^{2^n-1}$.

(ii) For $n \geq 6$, $\text{puso}(n) < 1.777128 \times 2^{2^n-1}$.

(iii) For $n = 2^k, k \geq 2$, $\text{puso}(n) \geq 2^{2^n-1-\log n+1}$.

This shows that the number $\text{puso}(n)$ is doubly exponential but still negligible compared to the number $\text{uso}(n)$ of USOs of the standard $n$-cube: Matoušek [13] has shown that

$$\text{uso}(n) \geq \left( \frac{n}{e} \right)^{2^n-1},$$

with a “matching” upper bound of $\text{uso}(n) = n^{O(2^n)}$.

As the main technical step, we count odd USOs. We start with the upper bound.
Lemma 23. Let $n \geq 1$. Then

(i) $\text{odd}(n) \leq 2\text{odd}(n-1)^2$ for $n > 0$.

(ii) For $n \geq 2$ and all $k < n$,

$$2\text{odd}(n-1) \leq (2\text{odd}(k))^{2^{n-1-k}} = 2^{k\sqrt{2\text{odd}(k)}2^{n-1}}. \quad (16)$$

Proof. By Corollary 17 (i), every odd USO consists of two odd USOs in two opposite facets, and edges along coordinate $n$, say, that connect the two facets. We claim that for every choice of odd USOs in the two facets, there are at most two ways of connecting the facets. Indeed, once we fix the direction of some connecting edge, all the others are fixed as well, since the orientation of an edge $\{V, V \oplus \{n\}\}$ determines the orientations of all “neighboring” edges $\{V \oplus \{i\}, V \oplus \{i, n\}\}$ via Corollary 17 (ii) (all 2-faces are bows). Inequality (i) follows, and (ii) is a simple induction.

The three bounds on $\text{puso}(n)$ now follow from $\text{puso}(n) = 2\text{border}(n-1)$ [7] and $\text{border}(n-1) = \text{odd}(n-1)$ [15]. For the bound of Theorem 22 (i), we use (16) with $k = 0$, and for Theorem 22 (ii), we employ $k = 5$ and $\text{odd}(5) = 44'075'264$. The lower bound of Theorem 22 (iii) is a direct consequence of the following “matching” lower bound on the number of odd USOs.

Lemma 24. Let $n = 2^k$, $k \geq 1$. Then $\text{odd}(n-1) \geq 2^{n-1-\log n}$.

Proof. If $n = 2^k$, there exists a perfect Hamming code of block length $n-1$ and message length $n-1-\log n$ [8]. In our language, this is a set $\mathcal{W}$ of $2^{n-1-\log n}$ vertices of the standard $(n-1)$-cube, with pairwise Hamming distance 3 and therefore disjoint neighborhoods. Hence, starting from the Klee-Minty cube $\text{KM}^{[n-1]}$, as introduced in Lemma 20, we can apply Lemma 21 to get a different odd USO for every subset of $\mathcal{W}$, by complementing all vertices in the given subset. The statement follows.

9 Conclusion

In this paper, we have introduced, characterized, and (approximately) counted three new classes of $n$-cube orientations: pseudo unique sink orientations (PU-OSOs), border unique sink orientations (facets of PU-OSOs), and odd unique sink orientations (duals of border USOs). A PUSO is a dimension-minimal witness for the fact that a given cube orientation is not a USO. The requirement of minimal dimension induces rich structural properties and a PUSO frequency that is negligible compared to the frequency of USOs among all cube orientations.
An obvious open problem is to close the gap in our approximate counting results and determine the true asymptotics of \( \log \text{odd}(n) \) and hence \( \log \text{puso}(n) \). We have shown that these numbers are between \( \Omega(2^{n-\log n}) \) and \( O(2^n) \). As our lower bound construction based on the Klee-Minty cube seems to yield rather specific odd USOs, we believe that the lower bound can be improved.

Also, border USOs and odd USOs might be algorithmically more tractable than general USOs. The standard complexity measure here is the number of outmap values\(^5\) that need to be inspected in order to be able to deduce the location of the sink \([20]\). For example, in dimension 3, we can indeed argue that border USOs and odd USOs are easier to solve than general USOs. It is known that 4 outmap values are necessary and sufficient to locate the sink in any USO of the 3-cube \([20]\). But in border USOs and odd USOs of the 3-cube, 3 suitably chosen outmap values suffice to deduce the orientations of all edges and hence the location of the sink \([18]\); see Figure 10.

\[ \]

Figure 10: The outmap values of the 3 indicated vertices determine the orientations of the bold edges. In the case of a border USO (left), the remaining orientations are determined by the condition that antipodal vertices have different outmap parities (Theorem 11). In the case of an odd USO (right), the remaining orientations are determined by the condition that all 2-faces are bows (Corollary 17(ii)).

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