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The corner poset with an application to an n-dimensional hypercube stacking puzzle

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Abstract

For any dimension $n \geq 3$, we establish the corner poset, a natural triangular poset structure on the corners of 2-color hypercubes. We use this poset to study a problem motivated by a classical cube stacking puzzle posed by Percy MacMahon as well as Eric Cross's more recent "Eight Blocks to Madness." We say that a hypercube is 2-color when each of its facets has one of two colors. Given an arbitrary multiset of 2-color unit n-dimensional hypercubes, we investigate when it is possible to find a submultiset of 2^n hypercubes that can be arranged into a larger hypercube of side length 2 with monochrome facets. Through a careful analysis of the poset and its properties, we construct interesting puzzles, find and enumerate solutions, and study the maximum size, $S(n)$, for a puzzle that does not contain a solution. Further, we find bounds on $S(n)$, showing that it grows as $\Theta(n2^n)$.

1 Introduction

Many classic puzzles provide a source of interesting mathematics in their analyses and solutions. A common theme is for the components of the puzzle to be colored in

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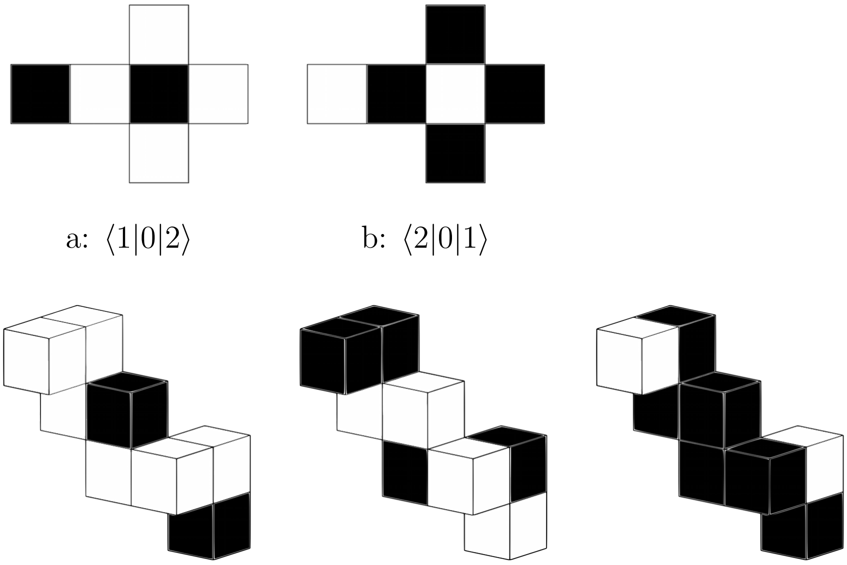
a particular way; the puzzle is solved when the components are arranged satisfying certain adjacency conditions. In this paper, we study a high-dimensional 2-color puzzle in this vein. In our case, a puzzle is a multiset consisting of n-dimensional unit hypercubes (*n-cubes*) with each facet colored from a fixed palette of two colors. We investigate when it is possible to find a solution to a given puzzle, i.e., a submultiset of 2^n hypercubes that can be arranged into a larger hypercube of side length 2 with monochrome facets. To do this, we determine how information about hypercube corners can be extracted from general coloring data. We show in Theorem 4.3 that the corner information provides a way to organize the collection of all 2-color hypercubes into a triangular poset structure, which we call the *corner poset*. We use properties of this poset to prove our other main results:

1. There is a polynomial time algorithm to determine if a puzzle has a solution, and we can enumerate solutions by counting lattice points in rational polyhedra (Proposition 5.1 and its subsequent material).
2. Largest multisets of n-cubes without solutions can be assumed to be composed of minimal n-cubes in the poset (Theorem 6.3).
3. The size, $S(n)$, of largest collections without solutions grows as $\Theta(n2^n)$ (Theorem 6.5), and we can give a non-trivial lower bound for an asymptotic constant (Proposition 6.7).

Our problem has its roots in a question of Alexander Percy MacMahon (1854–1929), a British mathematician who is known to number theorists for constructing tables of values of the partition function $p(n)$ and to combinatorialists for finding the generating function which enumerates a natural two-dimensional generalization of $p(n)$. MacMahon's interests also included recreational mathematics, and he created/patented several interesting puzzles [17]. One of those puzzles is a cube stacking problem which we now describe. Take six distinct colors and consider coloring the faces of a cube from this palette where each color appears exactly once. There are 30 ways of doing this up to rotation. MacMahon asked and answered the following question:

> *Given a cube in the* 6*-color collection, how can one construct a* $2 \times 2 \times 2$ *cube from* 8 *of the remaining* 29 *cubes which model the given cube (i.e., colors match the given cube on the outside) with colors also matching on the inside?*

John Horton Conway is given credit for finding a compact and elegant form of the complete solution to MacMahon's question above by arranging the 30 cubes of the 6-color collection into a certain 6×6 matrix with an empty diagonal. To solve MacMahon's original puzzle, one simply locates the given cube in the matrix, goes to its reflection (transpose entry), and then takes the eight other cubes in that row and column. See [15] for a more detailed discussion of Conway's matrix and [3] for



a: $\langle 1|0|2\rangle$ b: $\langle 2|0|1\rangle$

A: $\langle 1|0|3\rangle$ B: $\langle 2|0|2\rangle$ C: $\langle 3|0|1\rangle$

Figure 1: Some nets of 2-color cubes and hypercubes.

an analysis of the S_6-action on its rows. A variation of MacMahon's question was marketed as "Eight Blocks to Madness," released by Eric Cross in 1970 [9]. The Eight Blocks puzzle consists of eight unit cubes from the 6-color collection; the puzzle is solved by stacking the cubes into a $2 \times 2 \times 2$ cube, where each 2×2 face is a single color. This puzzle is analyzed in [14, 20], and its generalization is the subject of [11]. (For material on other stacking problems and their analysis, see [6], [8], [18], and [19].) Our puzzle has the same goal as the Eight Blocks puzzle, but we have two colors in an arbitrary dimension $n \geq 3$ and our puzzles can have more than 2^n blocks, some of which may not be used in any solution.

Each of our puzzles is a multiset of 2-color n-cubes, i.e., hypercubes in dimension n with each facet colored from a fixed palette of two colors. One obviously needs at least 2^n members in the multiset to solve the puzzle. On the other hand, any sufficiently large puzzle is guaranteed to have a solution by the pigeonhole principle, since there are finitely many types of 2-color n-cubes up to rotation, and once we have 2^n of any given type, we can build a scaled version of that n-cube. If, as above, $S(n)$ denotes the largest possible size of a multiset of cubes that *does not* contain a solution, then any puzzle of size $S(n)+1$ or larger will be guaranteed to have at least one solution. Puzzles with sizes in between 2^n and $S(n)$ are especially interesting because solutions may not exist at all and even when solutions do exist, they may not be easy to find or count.

Example 1.1. Consider the nets of some 2-color (black and white) cubes and 4-dimensional hypercubes in Figure 1. (The $\langle a|b|c\rangle$ notation in the figure will be introduced in Section 3 right before Corollary 3.3.) In general, a net is a polytope which has been unfolded in the next smallest dimension, like a box being flattened into a cross shape. In the case of cubes, the opposite faces in the net are clear since they correspond to opposite sides of the folded box. For the hypercube nets seen in Figure 1, the two black facets in "A" are opposite, the two white facets in "C" are opposite, and the remaining two pairs of opposite facets can be deduced from "B" (one pair black and one pair white). We can easily show, using the corner poset, that one cannot construct a $2 \times 2 \times 2$ solution given 7 "a" cubes, and 3 "b" cubes, nor a $2 \times 2 \times 2 \times 2$ solution given 15 "A," 7 "B," and 15 "C" hypercubes. This implies $S(3) \geq 7 + 3 = 10$ and $S(4) \geq 15 + 7 + 15 = 37$. In fact, $S(3) = 19$ and $S(4) = 53$. In the former case, a collection of 19 cubes without a solution consists of 7 each of monochrome black and white cubes, 2 "a" cubes, and 3 "b" cubes. Similar results for higher dimensions are summarized in Table 1.

We note that in a general cube stacking puzzle, finding the largest-sized puzzle without a solution depends on the number of colors used in the problem as well as the size of the $n \times n$ faces. In [5], it is shown that given any set of n^3 cubes having exactly 6 colors with $n > 2$, one can always construct an $n \times n \times n$ solution which models some k-color cube, i.e., one can arrange the n^3 cubes into a larger cube with colors matching the model cube on the outside and without restriction on the inside. Other variations of this problem appear in [2, 3, 4]. For the cases analogous to the $2 \times 2 \times 2$ Eight Blocks puzzle, there are sets of 10 cubes having exactly 2 colors without a solution [2]; 22 cubes having exactly 3 colors without a solution [2]; 10 cubes having exactly 4 colors without a solution [4]; and 23 cubes having exactly 6 colors without a solution [3, 11].

This paper is organized as follows. In Section 2, we provide preliminary notions and definitions. In Section 3, we count the number of 2-colorings of n-cubes up to rotation by analyzing color permutations induced by reflections, and show that the number and type of corners of a particular 2-color n-cube is completely determined by color pairs of opposite facets. In Section 4, we show how the corner types of different 2-color n-cubes give a well-defined partial order on the set of all 2-color n-cubes, and use that to build the corner poset. In Section 5, we apply results from the poset to determine algorithms for solving puzzles and enumerating solutions. We also show how the poset's structure implies the existence of interesting puzzles. In Section 6, we show how further analysis of the poset and its "upside-down" Pascal property give results on the composition and growth rate of the maximum multiset size without a puzzle solution.

2 Definitions and Conventions

When $n = 2$, our puzzle is straightforward to solve since it consists of four squares with colors on their boundary. Therefore, we will assume throughout this paper that $n > 2$ unless stated otherwise. The case $n = 3$, like the "Eight Blocks to Madness" puzzle, is already interesting. In the Eight Blocks puzzle, it is clear what is meant by orienting cubes so that each 2×2 face is of uniform color. In higher dimensions we need to be more careful, since it is not obvious what is meant by orienting a hypercube in $\mathbb{R}^n$, nor even how one should define a hypercube's coloring. We start by looking at particular substructures within the hypercube. We regularly embed an n-dimensional hypercube (which we will also refer to as an n-cube) for $n \geq 3$ into $\mathbb{R}^n$ centered about the origin so that every coordinate of each vertex is either 1 or -1. In this way our "unit cube" is actually a cube of side length 2. With this convention, we define a *facet* of a hypercube as the convex closure of all vertices that share a particular value, either 1 or -1, in a fixed coordinate; the facet corresponding to vertices with a 1 (or -1) in the ith coordinate is perpendicular to the ith coordinate axis. Therefore, an n-cube contains $2n$ facets. In any hypercube, there is a notion of facets which are *opposite*. These are two facets, one that has 1 in a fixed coordinate and the other that has -1 instead. *Opposite facets*, which we will also refer to as *opposite pairs*, are necessarily disjoint, since they are separated by some hyperplane $x_i = 0$. We note that any two facets in a hypercube are either opposite or they are *adjacent*, that is, their intersection is non-empty.

There are similar notions for vertices. Two vertices are *opposite* if none of their coordinates are equal or, equivalently, if each vertex is taken to the other via central inversion (changing the signs of all coordinates). We say two vertices are *adjacent* when they differ in exactly one coordinate so that they are joined by an edge in the hypercube. Unlike facets, however, vertices can be neither opposite nor adjacent, like the non-adjacent vertices on the square face of a cube.

Remark 2.1. We note that if v_1 and v_2 are opposite vertices, exactly one facet from every pair of opposite facets will contain v_1 and the other facet will contain v_2. In addition, given any two non-opposite facets, there is a vertex, either v_1 or v_2, that they both contain, and their opposite facets will contain the opposite vertex.

Next we describe what we mean by a coloring.

Definition 2.2. A *k-coloring* of an n-cube is a function from its $2n$ facets to a set of k-distinct elements, called *colors*.

A k-coloring of a cube includes the possibility that not all k colors appear in the range of the coloring function. When the function is surjective, we say that the coloring is *proper*.

One issue that arises in working with hypercube colorings is how to determine when two n-cube colorings are the same. Generally speaking, two colorings of n-cubes should be the same if there is a rotational symmetry in $\mathbb{R}^n$ that takes one to the other. The full group of symmetries of an n-dimensional hypercube or its dual the n-octahedron is known as a *hyperoctahedral group*. It is a Coxeter group of type B_n and can be described as the wreath product $S_2 \wr S_n = S_2^n \rtimes_\theta S_n$ where $\theta\colon S_n \to \mathrm{Aut}(S_2^n)$ is the natural homomorphism [10]. Consequently, the hyperoctahedral group in dimension n has order $2^n n!$. Since every coordinate of each hypercube vertex is either 1 or -1, symmetries of the hypercube are precisely the signed permutations of coordinates corresponding to the map θ above. The following collection is a (non-minimal) generating set of reflections for the hyperoctahedral group.

1. Reflections across a coordinate hyperplane $x_i = 0$. These are maps of the type r_i.

2. Reflections across the hyperplane $x_i = x_j$. These are maps of the type s_{ij}.

Here, r_i acts as multiplication by -1 in the ith coordinate while s_{ij} swaps the ith and jth coordinate. In the semidirect product $B_n = S_2^n \rtimes S_n$, the transpositions s_{ij} generate the factor S_n and the sign changes r_i generate the factor S_2^n. We are particularly interested in the index 2 subgroup $D_n \subset B_n$ consisting of elements that preserve orientation and correspond to rotations. Equivalently, those symmetries are the ones whose associated signed permutation matrix has determinant 1. Since the hyperoctahedral groups are reflection groups, we can also characterize the elements of D_n as those generated by an even number of reflections. We note that neither r_i nor s_{ij} are orientation preserving, so they are not elements of D_n.

We return to the question of when two hypercube colorings are the same. The n-cube symmetries we consider in this paper are compositions of reflections, so we need to determine the color permutations that a reflection might induce. A reflection of type r_i has the effect of swapping the colors on the opposite pair perpendicular to the coordinate axis x_i while leaving all other facets fixed. Reflections of type s_{ij}, on the other hand, exchange the opposite pairs that are perpendicular to the coordinate axes x_i and x_j while leaving all other facets fixed. (The reader may want to consider the cases of a square and a cube to get a sense of these color permutations.) We remark that the fixed facets are not fixed pointwise. Given a palette of k-colors, there is a natural equivalence relation on all k-colorings of a hypercube given by regarding two k-colorings as equivalent if one is obtained from the other by a rotation, i.e., an element of D_n. An equivalence class is called a *k-color n-cube*. In the next section we determine the total number of 2-color n-cubes.

We can now formally state, given a multiset of hypercubes, what it means to be able to solve our version of the cube stacking puzzle with $k = 2$ colors in an arbitrary dimension $n \geq 3$.

Definition 2.3. We call a multiset $\mathcal{P}$ of 2-color n-cubes a *puzzle*. We say that a submultiset of $\mathcal{P}$ consisting of 2^n n-cubes is a *solution* if there is a choice of corners, one from each n-cube in the submultiset, that can be put into a one-to-one correspondence with the corners of some hypercube H. In this case, we say that the solution is *modeled* on H.

We note that the assignment of corners means that the hypercubes in the solution can be arranged into a $2 \times 2 \times \cdots \times 2$ n-cube so that colors match along outer facets. However, as in the Eight Blocks puzzle, we do not require the restriction of MacMahon's puzzle that colors also match on the inside.

3 Characterizing 2-Color Hypercubes

In any 2-coloring of an n-cube, say with colors black (B) and white (W), the colors of opposite facets form either BB, BW, or WW unordered pairs. Clearly, any two 2-colorings that represent the same 2-color n-cube up to rotation determine the same number of each type of these BB, BW, or WW pairs. It turns out that the converse is also true.

Lemma 3.1. *If two 2-colorings of an n-cube have the same the number of BB, BW, and WW unordered pairs, then they represent the same 2-color n-cube, i.e., there is a rotation in D_n taking one 2-coloring to the other.*

Proof. It is sufficient to show that non-trivial color permutations of the facets induced by the generators r_i and s_{ij} can also be realized using elements of D_n. We start by showing that given a fixed 2-coloring of an n-dimensional hypercube, there is a rotation of the hypercube that has the effect of converting an ordered BW opposite pair into an ordered WB opposite pair while leaving all other colors fixed. This is the same non-trivial color permutation that is induced by a reflection r_i, and would justify treating the BW opposite pairs as unordered.

An ordered BW pair perpendicular to the coordinate axis x_i can be converted to an ordered WB pair while fixing all other faces by applying the transformation r_i. However, this reflection is orientation reversing. If there is some other opposite pair of type BB or WW associated to a coordinate j, then we can apply r_j, which does not change the relative position of any colors in the hypercube. The composition $r_j r_i$ has the desired effect and, since it is orientation preserving, is an element of D_n. The only remaining case is when all opposite pairs are of type BW. By Remark 2.1, it always happens that any two such opposite pairs will have their B facets containing some vertex v, while their opposite W facets will contain the opposite vertex $-v$. Let ρ be a rotation with $\rho(v) = (1, 1, 1, \ldots, 1)$. Then apply a map of type $\rho^{-1} s_{ij} \rho$ to swap these two BW pairs; the composition of the original mirror image with this map is orientation-preserving and has the desired effect. By iterating this procedure, we can construct a rotation in D_n which has the same effect on facet colors as interchanging any number of opposite pairs.

To complete the proof, we show that we can construct a rotation in D_n which induces the same color permutation as the reflection s_{ij} which exchanges any two pairs of opposite facets. First, we note that we can swap a BB or WW pair perpendicular to the coordinate axis x_i with any other opposite pair perpendicular to the axis x_j by using a reflection of type s_{ij}. We then follow it with a reflection of type r_i, which acts as the identity color permutation. The resulting composition is a rotation. The only remaining possibility is swapping two BW pairs, which was done in the first part of this proof. □

Remark 3.2. Lemma 3.1 is false in general for k-colorings with $k > 2$. Consider the two 3-color cubes in Figure 2 with colors black (B), white (W), and gray (G). These cubes have the same set of unordered pairs $\{BW, WG, GB\}$, but are mirror images which are not rotationally equivalent.

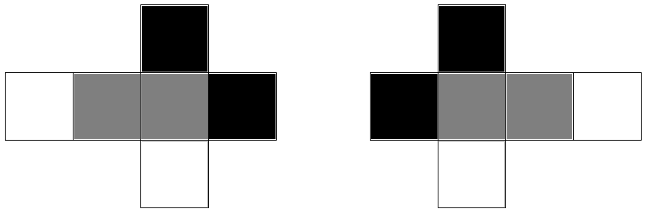


Figure 2: Mirror image 3-color cubes which are not rotationally equivalent.

Lemma 3.1 tells us that a 2-color n-cube is completely determined by its opposite pairs. If the number of BB, BW, and WW pairs are a, b, and c, respectively, then we use the notation $\langle a|b|c\rangle$ to denote this 2-color n-cube. For examples of this notation, see Figure 1 in the introduction.

Corollary 3.3. *There are $\binom{n+2}{2}$ 2-colorings of n-cubes up to rotation.*

Proof. There are $\binom{n+2}{2}$ multisets of size n using three distinct elements. □

Another result related to Lemma 3.1 concerns the classification of corners of a hypercube. The *corner type* of a vertex v in a k-coloring of a hypercube can be defined as follows. Rotate v to the vertex $(1, 1, 1, \dots, 1)$ and consider the sequence of colors of the facets corresponding to $(1, *, *, \dots, *)$, $(*, 1, *, \dots, *)$, $\dots$, $(*, *, \dots, *, 1)$, where $*$ consists of all values in the interval $[-1, 1]$. The corner type of v is then the equivalence class of all such sequences resulting from different choices of rotations taking v to $(1, 1, \dots, 1)$.

Proposition 3.4. *If $k < n$, then the corner type of a vertex in a k-coloring of an n-cube is completely determined by the multiset of colors coming from facets containing that vertex.*

Proof. Recall that we assume $n \geq 3$. We fix a vertex v in the hypercube and rotate it to $(1, 1, \dots, 1)$. From the characterization of symmetries as signed permutations, we see that the stabilizer of $(1, 1, \dots, 1)$ in D_n, the subgroup of rotations, is isomorphic to the alternating group A_n. In particular, every element of this stabilizer can be written as the composition of an even number of reflections of the form s_{ij}. Since $k < n$, there are 2 facets around $(1, 1, \dots, 1)$ which have the same color. A reflection $\hat{\sigma}$ of the form s_{ij} which swaps these facets does not change the sequence of colors adjacent to v. Now take an element σ of S_n, the stabilizer of $(1, 1, \dots, 1)$ in B_n, corresponding to some permutation of coordinates. If σ can be written as the composition of an even number of transpositions s_{ij}, then it is in D_n. If not, $\sigma\hat{\sigma}$ is an element of D_n whose effect as a color permutation on the facets containing $(1, 1, \dots, 1)$ is identical to σ. Thus, any color permutation of the facets containing v can be realized from a rotation from D_n. □

Remark 3.5. Proposition 3.4 does not hold when the number of colors, k, is equal to or greater than n. For example, see Figure 2. There is no rotation in D_3 which takes the corner type GWB (read counterclockwise) to the corner type GBW. The reader may wish to compare Proposition 3.4 with Lemma 3.1.

4 The Corner Poset of Hypercubes

When constructing an n-cube of side length 2 from 2^n n-cubes of unit length, some hypercubes are more flexible than others. What we mean is that a hypercube with many different corners can be used in more potential positions in a solution than a hypercube with fewer of them. As a way of understanding more about an n-cube's collection of corners, we start with a result that connects the colors that appear at a corner, the *color type* of the corner, to the collection of opposite pairs of the n-cube.

Proposition 4.1. *Let a, b, and c be the number of BB, BW, and WW opposite pairs, respectively, in a fixed hypercube H, i.e., $H = \langle a|b|c\rangle$. Then the generating function for the color types of H is given by*

$$(B+B)^a(B+W)^b(W+W)^c = \sum_{k=0}^{b} 2^{a+c}\binom{b}{k}B^{a+k}W^{c+b-k}. \tag{1}$$

Proof. A choice of facet color from each opposite pair determines a color at a corner. The formula on the right follows from noting

$$(B+B)^a(B+W)^b(W+W)^c = 2^{a+c}B^aW^c(B+W)^b.$$

□

We note that Proposition 4.1 easily generalizes to n-cubes with any number of colors. In addition, when $k < n$, Proposition 3.4 implies that the corner type of a vertex is determined by its color type. This, along with the observation that $(B+W)^b$, contains $b+1$ terms, yields the following corollary.

Corollary 4.2. *Let $n > 2$, and let a, b, and c be the number of BB, BW, and WW opposite pairs, respectively, in a fixed 2-color n-dimensional hypercube H, i.e., $H = \langle a|b|c\rangle$. Then the generating function for the corner types of H is given by Equation (1). Further, the number of distinct corner types in H is one more than the number of BW opposite pairs it contains.*

Given hypercubes H_1 and H_2, we say $H_2 \preceq H_1$ if every corner of H_2 is also a corner of H_1, ignoring multiplicity[1]. The relation $\preceq$ is obviously reflexive and transitive. Corollary 4.2 also implies that $\preceq$ is antisymmetric, since if $H_1 \preceq H_2$ and $H_2 \preceq H_1$, both n-cubes have the same number of BW opposite pairs. Consequently,

[1]We need not be concerned with multiplicity since at most one corner from a sub-cube is visible in the construction.

their generating functions are the same, and H_1 and H_2 are the same up to rotation by Lemma 3.1. Therefore, $\preceq$ defines a partial order on the 2-color n-cubes. We would like to understand the resulting corner poset.

Theorem 4.3. *When $n > 2$, the set of 2-color n-cubes forms a poset under $\preceq$. In particular, given an n-cube with at least one BW pair, there are two 2-color n-cubes directly below it in the poset, the ones that result from replacing the BW opposite pair with either a WW or BB opposite pair.*

Proof. By Corollary 4.2, the number of corner types of an n-cube is determined by the number of its BW opposite pairs. Assume we have an n-cube H_1 with b BW opposite pairs. If we replace one of those opposite pairs with a monochrome opposite pair, then the resulting 2-color n-cube, H_2, is uniquely determined by Lemma 3.1. Furthermore, H_2 has exactly $b - 1$ BW opposite pairs. We note that every corner of H_2 is also a corner of H_1, i.e., $H_2 \preceq H_1$. Given a choice of colors from the $b - 1$ BW opposite pairs of H_2, the same colors can be chosen from $b - 1$ BW pairs from H_1. Since in H_1 there are two color choices for the bth opposite pair, we can match any color choice for the new monochrome opposite pair in an appropriate corner. The remaining $n - b$ opposite pairs are of type BB and WW, and have the same multiplicity in both H_1 and H_2. The result follows by Proposition 3.4. $\square$

Using the notation preceding Corollary 3.3, we refer to elements in the poset by their triple $\langle a|b|c\rangle$ of BB, BW, and WW opposite pairs. We note that the corner poset contains a unique maximal element, $H_{max} = \langle 0|n|0\rangle$. This is the unique 2-color n-cube whose opposite pairs are all of type BW, and it contains all possible corner types. On the other hand, there are $n + 1$ minimal elements in the poset having zero opposite pairs of type BW. In addition, we move down the poset by replacing an BW opposite pair with a monochrome opposite pair. This means that the poset has the form of a triangle, and the hypercubes in each row are determined by the number of BW pairs they contain. We refer to the row of the poset which contains the n-cubes of the form $\langle *|k|n-(*+k)\rangle$ as row k. Finally, each non-minimal element in the poset covers two other elements, and it is straightforward to see from the characterization in Theorem 4.3 that each non-maximal element is covered by either one or two other elements, depending on whether it contains one or both of the BB and WW opposite pairs. For example, consider the poset for $n = 4$, given in Figure 3. As noted by an anonymous referee, the corner poset is the interval poset on the chain of $n + 1$ elements, given by the number of white facets adjacent to a vertex.

The corner types of minimal 2-color n-cubes in the poset have particularly simple forms.

Corollary 4.4. *The 2^n vertices of minimal 2-color n-cubes in the poset are all of the same corner type.*

Proof. From Corollary 4.2 as well as Theorem 4.3 and the discussion afterwards, minimal 2-color n-cubes in the poset contain no BW opposite pairs and have the

$$\begin{tikzcd}[column sep=tiny]
 & & & & \langle 0|4|0\rangle \arrow[dl] \arrow[dr] & & & & \\
 & & & \langle 0|3|1\rangle \arrow[dl] \arrow[dr] & & \langle 1|3|0\rangle \arrow[dl] \arrow[dr] & & & \\
 & & \langle 0|2|2\rangle \arrow[dl] \arrow[dr] & & \langle 1|2|1\rangle \arrow[dl] \arrow[dr] & & \langle 2|2|0\rangle \arrow[dl] \arrow[dr] & & \\
 & \langle 0|1|3\rangle \arrow[dl] \arrow[dr] & & \langle 1|1|2\rangle \arrow[dl] \arrow[dr] & & \langle 2|1|1\rangle \arrow[dl] \arrow[dr] & & \langle 3|1|0\rangle \arrow[dl] \arrow[dr] & \\
\langle 0|0|4\rangle & & \langle 1|0|3\rangle & & \langle 2|0|2\rangle & & \langle 3|0|1\rangle & & \langle 4|0|0\rangle
\end{tikzcd}$$

Figure 3: Poset structure of 2-color 4-cubes.

form $\langle a|0|c\rangle$. Therefore, all 2^n corners of these n-cubes have a facets colored B and c facets colored W, with $a + c = n$. The result follows from Proposition 3.4 and Corollary 4.2. □

Remark 4.5. The anti-symmetry of $\preceq$ fails in general for more than two colors. An example is given by the two 3-cubes, H_1 and H_2, from Figure 2 in Section 3. They have the same corner types but are mirror images of each other and so are not rotationally equivalent. Therefore, $H_1 \preceq H_2$ and $H_2 \preceq H_1$, but H_1 and H_2 are not rotationally equivalent.

5 Solving and Constructing Puzzles

The results in Section 3 and Section 4 give us a way to describe and compare hypercubes. In this section, we apply those results to our cube stacking puzzle. From Definition 2.3 in Section 2, we can consider a solution as a matching between a submultiset of $\mathcal{P}$ of size 2^n and a collection of corners corresponding to some 2-color n-cube to be modeled. We will use this formulation to show that it is possible to determine whether $\mathcal{P}$ has a solution in polynomial time with respect to the size of $\mathcal{P}$.

We start with an observation between hypercubes and their corners which appear in the poset. By Corollary 4.4, the n-cubes in the bottom of the poset have just one type of corner, so we can identify a corner with its corresponding n-cube in row 0. Specifically, in dimension n, we will refer to the unique corner of $\langle k|0|n-k\rangle$ as corner k. The poset also gives us a way to visualize the corners of an n-cube—these are the corners that lie in the triangular cone below the n-cube. For example, consider the position marked “4” in Figure 4, which is the 3-cube $\langle 0|2|1\rangle$. Following its cone to the bottom of the poset and again applying Corollary 4.2, we see that the 3-cube has two each of corners 1 and 3, and four of corner 2. We can represent this corner set as $[2, 4, 2, 0]$. In general, Corollary 4.2 implies that the n-cube $\langle a|b|c\rangle$, where

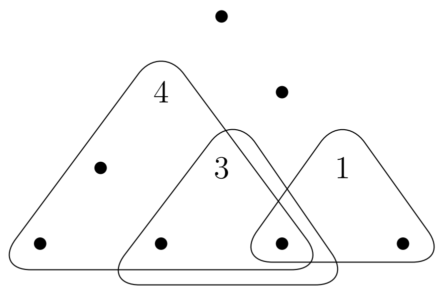


Figure 4: Hypercube corners and puzzle solutions with $n = 3$, showing four copies of $\langle 0|2|1\rangle$, three copies of $\langle 1|1|1\rangle$, and one copy of $\langle 2|1|0\rangle$.

$a + b + c = n$, has corner set

$$2^{a+c}[\underbrace{0,\ldots,0}_{a\text{ copies}}, \binom{b}{0}, \binom{b}{1}, \ldots, \binom{b}{b}, \underbrace{0,\ldots,0}_{c\text{ copies}}]. \tag{2}$$

Proposition 5.1. *There is a polynomial time algorithm to determine if a puzzle $\mathcal{P}$ has a solution.*

Proof. Given a fixed 2-color n-cube H, we can determine if $\mathcal{P}$ has a solution that is modeled on H by recasting the puzzle as a bipartite matching problem. Add a vertex in one bipartition for each n-cube in $\mathcal{P}$. The other bipartition will have 2^n vertices, one each for each corner of H, including multiplicity. We connect a vertex in the first bipartition with a vertex in the second bipartition if the n-cube in $\mathcal{P}$ has the corresponding corner in H. A solution in this context is a matching of size 2^n, that is, 2^n cubes in $\mathcal{P}$ which can be placed in appropriate corner positions of the larger hypercube modeled on H.

Recall from the introduction that a puzzle with fewer than 2^n hypercubes will never have a solution, and any puzzle with $\binom{n+2}{2}(2^n - 1) + 1$ or more hypercubes will always have one by Corollary 3.3 and the pigeonhole principle. Thus, if we set $m = 2^n$, we may assume that our puzzles are $O(m(\log m)^2)$ in size. Therefore, we can encode every puzzle as a bipartite graph with $O(m(\log m)^2)$ vertices. Since each cube can match with up to $2^n = m$ corners, the graph will have $O(m^2(\log m)^2)$ edges. By a result of Hopcroft and Karp ([13]), one can find a maximum matching in a bipartite graph with $|V|$ vertices and $|E|$ edges in $O(\sqrt{|V|}|E|)$ time. In our matching problem, this corresponds to $O(m^{2.5}(\log(m))^3)$ time to determine if there is a matching of size 2^n. Finally, we may need to perform this matching for all $\binom{n+2}{2}$ possible n-cubes, resulting in an algorithm that runs in $O(m^{2.5}(\log(m))^5)$ time. □

We next describe how to enumerate puzzle solutions. The algorithm outlined in Proposition 5.1 will find a solution to $\mathcal{P}$ if it exists, and it may find many. However, a matching may not distinguish cases that we would like to be considered the same, say when two identical 2-color n-cubes are assigned to two identical corners. We note that the matching in Proposition 5.1 sends multisets of 2-color n-cubes to multisets of corners. We will consider two such matchings, M_1 and M_2, to be equivalent if both associate to each type of n-cube the same number and type of corners.

We outline a procedure one can follow to determine the total number of non-equivalent puzzle solutions that are modeled on a particular 2-color n-cube. In the dimension n setting, there are $\binom{n+2}{2}$ different n-cubes, which we enumerate using i, and $n+1$ possible corner types, which we enumerate using j. Given a puzzle, let $d_i \geq 0$ be the number of copies of the n-cube i in $\mathcal{P}$. Define a_{ij} to equal 1 if cube i has corner j and 0 otherwise. To determine if a puzzle has solutions that look like some fixed 2-color n-cube H, define b_j to be the number of corners of type j in H; the values of b_j, which follow from Corollary 4.2, are binomial coefficients scaled by some non-negative power of 2. Finally, define the variables we wish to solve for, $\{x_{ij}\}$, to be the number of n-cubes i which are used for corner j in the solution.

In order to model this fixed 2-color n-cube H, we have the following system of equations and inequalities:

1. For all j:
$$\sum_{i=1}^{\binom{n+2}{2}} a_{ij} x_{ij} = b_j.$$
This says that enough cubes have been assigned to match with all requisite corners of type j.

2. For all i:
$$\sum_{j=0}^{n} x_{ij} \leq d_i.$$
This says that we did not assign the n-cube of type i to more corners than there are copies in $\mathcal{P}$.

3. For all i, j:
$$x_{ij} \geq 0.$$
This says we did not assign a negative number of n-cubes at any point.

4. To avoid extraneous solutions, we require
$$\sum_{i,j} x_{ij} = 2^n.$$
This ensures that all of the variables which did not appear in an equation with a nonzero b_j become zero since we also have $b_0 + b_1 + \cdots + b_n = 2^n$.

Since the equations are all hyperplanes and the inequalities are all half-spaces, the solution space when regarding all x_{ij} as real variables is a convex set. Each integer lattice point in the solution space can be identified with a solution to the puzzle modeled on H, up to equivalence. In two dimensions, the number of lattice points in such a region can be counted using Pick's Theorem. The analogous problem in the higher dimensional setting can be solved using Barvinok's algorithm. (See [1], for example, or its implementation in LattE [16].) As in the proof of Proposition 5.1, one needs to consider each of the $\binom{n+2}{2}$ hypercube cases separately to fully enumerate all solutions. Although the solution space to implement Barvinok's algorithm appears to live in a large dimension compared to n, the minimum number of variables needed in a particular case can actually be smaller than it might appear at first.

Example 5.2. Suppose, in dimension $n = 3$, that we are trying to find how many ways we can model $H = \langle 0|1|2\rangle$ having corner set $[b_0, b_1, b_2, b_3] = [4, 4, 0, 0]$ from a puzzle $\mathcal{P}$ consisting of $d_1 = 3$ copies of H, $d_2 = 5$ copies of $\langle 1|1|1\rangle$ with corner set $[0, 4, 4, 0]$, and $d_3 = 4$ copies of $\langle 0|2|1\rangle$ with corner set $[2, 4, 2, 0]$. We have the following system of equations and inequalities on variables $x_{ij} \geq 0$:

$$\begin{aligned} x_{10} + x_{30} &= 4 \\ x_{11} + x_{21} + x_{31} &= 4 \\ x_{10} + x_{11} &\leq 3 \\ x_{21} &\leq 5 \\ x_{30} + x_{31} &\leq 4 \\ \sum_{i,j} x_{ij} &= 8. \end{aligned}$$

All variables not appearing in the first five lines can be ignored since they are forced to be zero. We can use the equations to eliminate the variables x_{30} and x_{31} as long as we ensure the quantities representing them remain nonnegative. If we set $x = x_{10}$, $y = x_{11}$, and $z = x_{21}$, then after removing redundancies we get the system of inequalities

$$\begin{aligned} x + y &\leq 3 \\ y + z &\leq 4 \\ x + y + z &\geq 4 \\ y &\geq 0. \end{aligned}$$

These cut out a tetrahedral region in xyz-space seen in Figure 5. The 20 lattice points in the region correspond to 20 distinct ways of building H from our puzzle $\mathcal{P}$.

In general, a "good puzzle" should contain many hypercubes with lots of different corners, and many choices of corner orientations. That way, the solver will have many choices of which corners to incorporate as well how to orient them in the final solution. We see that n-cubes higher up in the poset have more distinct types of corners, whereas n-cubes towards the bottom of the poset have fewer. We remark that although the cube $\langle k|0|n-k\rangle$ has only one type of corner, that corner has $\binom{n}{k}$ possible orientations, so that a puzzle with many n-cubes that are lower in the poset can still be challenging. Another possible desirable puzzle property may be for it to have a unique solution.

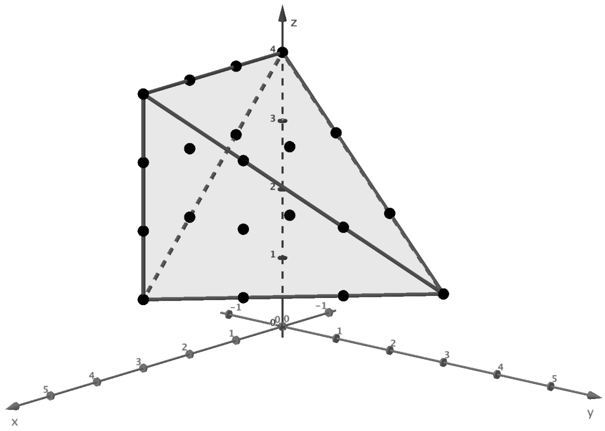


Figure 5: Lattice points in tetrahedral region for Barvinok's algorithm.

Example 5.3. Consider the puzzle in Figure 4, with four copies of $\langle 0|2|1\rangle$, three copies of $\langle 1|1|1\rangle$, and one copy of $\langle 2|1|0\rangle$. We note that the corners $[1, 0, 0, 0]$ and $[0, 0, 0, 1]$ are monochrome, whereas the other two corners, $[0, 1, 0, 0]$ and $[0, 0, 1, 0]$, can be oriented three ways. This eight-cube puzzle has seven distinct solutions, representing three distinct corner sets: $[1, 3, 3, 1]$, $[2, 4, 2, 0]$ (two different ways), and $[0, 4, 4, 0]$ (four different ways). These are the 3-cubes $\langle 0|3|0\rangle$, $\langle 0|2|1\rangle$, and $\langle 1|1|1\rangle$, respectively. Because there are so many possible solutions, this might not be an ideal puzzle. However, if the copy of $\langle 2|1|0\rangle$ in the puzzle is replaced by a copy of $\langle 3|0|0\rangle$, then there is only one solution, the 3-cube $\langle 0|3|0\rangle$. In this case there are still many possible configurations for the puzzle solver to consider. There are

$$\frac{\left(\binom{8}{4}3^4\right)\left(\binom{4}{3}2^3\right)}{4!} = 7560$$

ways, up to rigid rotation, to put the cubes into position and choose a corner to face outward, and this count does take into account orientating the corners. However, the puzzle may still not be challenging from a puzzle solver's standpoint.

One aspect that impacts this puzzle's difficulty is the presence of the monochrome cube $\langle 3|0|0\rangle$. There is no corner choice in its use, and it also restricts which cubes can be adjacent to it as well as their orientation. Puzzles can be made more challenging by using cubes that are not in the lowest rows of the poset. We will show that for a large enough n, it is possible to build puzzles of this type. In particular, challenging puzzles live in high dimensions.

Proposition 5.4. *Fix an integer $\ell \geq 1$. For n sufficiently large, it is possible to build a puzzle with a unique solution that does not use cubes from the first ℓ rows of the poset.*

Proof. Let $n = 3(\ell+1)-1 = 3\ell+2$, and consider the puzzle $\mathcal{P}$ containing 2^n n-cubes, distributed as three sets, $\sum_{i=0}^{\ell} \binom{n}{i}$ copies of n-cubes $\langle 0|\ell|2\ell+2\rangle$ and $\langle 2\ell+2|\ell|0\rangle$, and $\sum_{i=\ell+1}^{2\ell+1} \binom{n}{i}$ copies of n-cube $\langle \ell+1|\ell|\ell+1\rangle$. This puzzle is illustrated in Figure 6. By

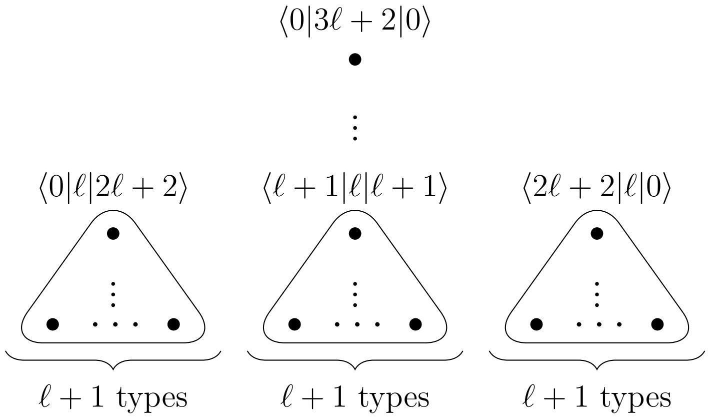


Figure 6: "High row" puzzles with a unique solution.

using $\binom{n}{i}$ copies of the appropriate cube for the corner types represented by the ith entry of the bottom row, Equation 2 implies that we have precisely the corner types needed to model a solution of type $\langle 0|n|0\rangle$.

We claim that $\langle 0|n|0\rangle$ is the only possible solution to this puzzle. Note that the corner types for these three sets are mutually disjoint and there are the same number of cubes of type $\langle 0|\ell|2\ell+2\rangle$ and $\langle 2\ell+2|\ell|0\rangle$. These observations imply that the only possible solutions to $\mathcal{P}$ are of the form $\langle k|n-2k|k\rangle$, with $k > \ell+1$. We will show that the $\sum_{i=0}^{\ell}\binom{n}{i}$ copies of the cubes of type $\langle 0|\ell|2\ell+2\rangle$ cannot be used as corners in any other of these solutions. This fact follows from the following observation about binomial coefficients.

$$\begin{aligned}
\binom{n}{0}+\cdots+\binom{n}{\ell} &= 2\left(\binom{n-1}{0}+\cdots+\binom{n-1}{\ell-1}\right)+\binom{n-1}{\ell} \\
&= 2\left[2\left(\binom{n-2}{0}+\cdots+\binom{n-2}{\ell-2}\right)+\binom{n-2}{\ell-1}\right]+\binom{n-1}{\ell} \\
&= 2\left[2\left(\binom{n-2}{0}+\cdots+\binom{n-2}{\ell-1}\right)\right]+\binom{n-1}{\ell}-2\binom{n-2}{\ell-1} \\
&= 2^2\left(\binom{n-2}{0}+\cdots+\binom{n-2}{\ell-1}\right)+\binom{n-2}{\ell}-\binom{n-2}{\ell-1}.
\end{aligned}$$

As $\ell < \frac{n}{2}$, the unimodality of binomial coefficients implies that $\binom{n-2}{\ell}-\binom{n-2}{\ell-1} > 0$. Comparing this with Equation 2, we see that there are $\binom{n-2}{\ell}-\binom{n-2}{\ell-1}$ cubes too many of type $\langle 0|\ell|2\ell+2\rangle$ to use for appropriate corners of a solution modeled on $\langle 1|n-2|1\rangle$, which implies that the latter is not a solution to $\mathcal{P}$. Iterating this process proves that $\langle 0|n|0\rangle$ is the sole solution.

It is important to split the bottom row into thirds in this construction. If $n = 2\ell+1$, then $\sum_{i=0}^{\ell}\binom{n}{i} = 2^{n-1}$, and one can use 2^{n-1} copies of $\langle \ell|0|\ell+1\rangle$ and $\langle \ell+1|0|\ell\rangle$ to construct a solution that looks like $\langle \ell|1|\ell\rangle$. □

We remark that the collection described in Proposition 5.4, because of its symmetry, size, and uniqueness of solution, would probably be an interesting and challenging puzzle to solve by trial and error. On the other hand, it is also interesting to consider puzzles with many solutions. Borrowing from [11], given a subset $\mathcal{H}$ from the set of all 2-color n-cubes, we say a puzzle $\mathcal{P}$ is *$\mathcal{H}$-complete* if the solution set of $\mathcal{P}$ is precisely $\mathcal{H}$. Can we always construct a puzzle which is $\mathcal{H}$-complete for any $\mathcal{H}$? Haraguchi answered this question in the negative for a generalization of the Eight Blocks puzzle and found a minimal puzzle which was complete with respect to the set of all 30 proper 6-color 3-cubes [11]. In our case, the answer is clearly no as well since if a puzzle can model two adjacent minimal n-cubes $\langle i|0|n-i\rangle$ and $\langle i+1|0|n-i-1\rangle$, then the puzzle can also model $\langle i|1|n-i-1\rangle$. It is also possible to find a puzzle which is complete with respect to all 2-color n-cubes; for example, consider the puzzle consisting of 2^n copies of $\langle 0|n|0\rangle$ (top n-cube in the corner poset). In the other extreme, given any 2-color n-cube H, we can always find a puzzle which is $\{H\}$-complete by considering the multiset of minimal 2-color n-cubes corresponding to the corners of H as in Corollary 4.2. We also note that if we can construct any number of consecutive entries in row 0 of the poset, then we can construct any entry in the triangular cone above the consecutive entries. In a different but related vein, given 2^{n-1} copies of any two n-cubes H_1 and H_2, we can construct any entry which lies in the intersection of the triangular cones below H_1 and H_2 as in Figure 4. A full analysis and characterization of $\mathcal{H}$-complete puzzles could be a worthwhile future project.

6 Maximal Sets Without Solutions

In this section, we investigate necessary conditions associated to solutions and non-solutions to our puzzle.

Definition 6.1. Let $S(n)$ denote the size of a largest collection of n-cubes such that no subset of that collection is a solution.

As noted in the introduction, the pigeonhole principle implies that $S(n)$ exists and is well-defined. To learn a bit more about the values of $S(n)$, we start with a result that tells us that we can restrict the 2-color n-cubes that we consider. To state the result, we first need a definition.

Definition 6.2. Given puzzles $\mathcal{P}_1$ and $\mathcal{P}_2$, we write $\mathcal{P}_1 \preceq \mathcal{P}_2$ to indicate that there is a bijection $H \mapsto H'$ from the multiset $\mathcal{P}_1$ to a submultiset of $\mathcal{P}_2$ such that $H \preceq H'$ for all H in $\mathcal{P}_1$.

Theorem 6.3. *A puzzle $\mathcal{P}$ has a solution if and only if there is a puzzle $\widetilde{\mathcal{P}} \preceq \mathcal{P}$ of the same size with a solution and containing only minimal 2-color n-cubes. Therefore, the value of $S(n)$ can be realized by a puzzle consisting entirely of minimal 2-color n-cubes in the corner poset.*

Proof. Suppose we can build a solution from 2-color n-cubes in $\mathcal{P}$. Then each n-cube H in the solution is used solely for a particular corner. We can replace H with the unique minimal 2-color n-cube $\widetilde{H} \preceq H$ whose corners all have that corner type and use $\widetilde{H}$ in place of H in the solution. We can similarly replace the other n-cubes in $\mathcal{P}$ not used in the solution with minimal n-cubes below them in the poset. The resulting puzzle $\widetilde{\mathcal{P}} \preceq \mathcal{P}$ will have a solution and will be the same size as $\mathcal{P}$, but with all minimal 2-color n-cubes.

Now take any puzzle $\mathcal{P}$ of 2-color n-cubes *without* a solution. Let $\widetilde{\mathcal{P}}$ be any puzzle obtained by replacing each 2-color n-cube H in $\mathcal{P}$ with a minimal 2-color n-cube $\widetilde{H} \preceq H$ in the poset. Note that the corner type of $\widetilde{H}$ is also a corner type of H. Thus $\widetilde{\mathcal{P}} \preceq \mathcal{P}$ does not have a solution because if we could build a solution from n-cubes in $\widetilde{\mathcal{P}}$, then we could build a solution with the original puzzle $\mathcal{P}$. This finishes the proof of the proposition since $|\mathcal{P}| = |\widetilde{\mathcal{P}}|$. □

We have established a significant reduction: by Corollary 4.4 and Theorem 6.3, we may represent a puzzle $\mathcal{P}$ by a vector $(a_0, a_1, \ldots, a_n)$, where each a_i is the multiplicity of the minimal 2-color n-cube $\langle i|0|n-i\rangle$. Corollary 4.4 and Theorem 6.3 together also imply that in a puzzle $\mathcal{P}$, we can identify a minimal cube in the multiset with the corner type it is matched to in the solution. If a puzzle $\mathcal{P}$ of n-cubes does not have a solution, this means that we cannot construct any of the 2-color n-cubes in the poset. By Corollary 4.2, we know the number and corner type of every vertex of every 2-color n-cube. Each 2-color n-cube can be translated into a constraint that the elements of $\mathcal{P}$ must satisfy. We construct these next.

There are $n+1$ 2-color n-cubes on the bottom row of the poset (recall from Theorem 4.3 that this is row 0, matching the number of BW opposite pairs), and these are all minimal. Therefore, if $\mathcal{P} = (a_0, a_1, \ldots, a_n)$ does not have a solution, the $n+1$ inequalities $a_i \leq 2^n - 1$ for $i = 0, 1, \ldots n$ must be satisfied. We set the constraint $C_{0,i}$ to be the condition $a_i \leq 2^n - 1$. We do something similar with row 1 (second from the bottom, one BW opposite pair): the 2-color n-cubes in that row have two corner types, each with multiplicity 2^{n-1}. The resulting n constraints each have the form of a disjunction

$$C_{1,i} : \left(a_i \leq 2^{n-1} - 1\right) \vee \left(a_{i+1} \leq 2^{n-1} - 1\right)$$

for $i = 0, 1, \ldots, n-1$. In general, there are $n+1-k$ n-cubes in row k of the poset. By Corollary 4.2, each 2-color n-cube in row k has $k+1$ distinct corner types, and each corner type appears $2^{n-k}\binom{k}{j}$ times, for some $0 \leq j \leq k$. Therefore, the constraint associated to the first 2-color n-cube of row k is

$$C_{k,0} : \bigvee_{j=0}^{k} \left(a_j \leq 2^{n-k}\binom{k}{j} - 1\right). \tag{3}$$

The constraints $C_{k,i}$ with $0 < i \leq n-k$ are defined analogously. In order for $\mathcal{P}$ to not have a solution, the conjuction of the constraints

$$\bigwedge_{k=0}^{n} \bigwedge_{i=0}^{n-k} C_{k,i} \tag{4}$$

must be satisfied.

Lemma 6.4. *The value of $S(n)$ is maximized for some puzzle of the form $\mathcal{P} = (a_0, a_1, \ldots, a_n)$, where each a_i has the form $2^r\binom{s}{t} - 1$.*

Proof. Every literal in Equation (3) has the form $a_i \leq 2^r\binom{s}{t} - 1$, and the choice of a value for a_i will determine the truth of each literal of which it is part. If the initial value of a_i makes a literal false, then increasing its value will not change the truth of the literal. So consider all literals where the value of a_i makes the literal true. There are finitely many, and all of the literals are integer inequalities. Therefore, we can increase the value of a_i up to the value where the most restrictive inequality remains true. Changing the value of a_i in this way will not affect the overall truth of Equation (4). □

Lemma 6.4 suggests one way to find the value of $S(n)$. One enumerates the possible values for a_i in literals in Equation (4), then searches through all choices of $(a_0, a_1, \ldots, a_n)$ to find the maximum sum of the coefficients such that Equation (4) is false—these are puzzles $\mathcal{P}$ of largest size without solutions. We thank Frank Xia, who coded this search routine into C++ and generated the results in Table 1 up to dimension $n = 14$. We remark that we referenced the $n = 3$ and 4 cases in the introduction. The table includes the best known values for $S(n)$. The explicit search shows that generally there is more than one puzzle of minimum size. We denote the total number of such puzzles by $T(n)$, using an asterisk to denote cases which are conjectural. Some of these puzzles arise by symmetry, since if $(a_0, a_1, \ldots, a_n)$ is a puzzle of maximum size, then so is $(a_n, a_{n-1}, \ldots, a_0)$. However, consider $(31, 15, 31, 3, 31, 15)$ and $(31, 11, 31, 7, 15, 31)$, which are non-equivalent puzzles without solutions when $n = 5$. In the cases $n = 11, 12, 13$, a search was conducted assuming that the values of a_0 and a_n were as large as possible, hence the inequality. (We believe this is usually true, although recall the given examples from the $n = 5$ case where this does not happen.)

This naive search routine works for small values of n, but a back-of-the-envelope calculation shows why this procedure will not work for long. The number of literals in Equation (4) is $\sum_{k=0}^{n}(k+1)(n+1-k)$; a quick computation shows that this sum is about $\frac{n^3}{6}$, so the average number of choices for each a_i is about $\frac{n^2}{6}$. Therefore, finding the optimal value of $S(n)$ through an exhaustive search requires checking roughly $O\left((n^2)^n\right)$ cases. Further, Equation (4) can be readily rewritten in conjunctive normal form, and it is known that general satisfiability of these expressions is an NP-complete problem by Cook's theorem [7].

On the other hand, we can get some general results on the growth rate of $S(n)$.

Theorem 6.5. *We have $S(n) = \Theta(n2^n)$. In particular,*

$$\left\lfloor \frac{n+2}{2} \right\rfloor (2^n - 1) \leq S(n) \leq (n+1)\left(\frac{3}{4} \cdot 2^n - 1\right) + 2^{n-2}.$$

Proof. We will show the inequalities follow from Equation (2) and Lemma 6.4. The left inequality follows from considering puzzles of the form $(2^n - 1, 0, 2^n - 1, 0, \ldots)$.

n	$S(n)$	Sample Largest Known Puzzle without a Solution	$T(n)$
2	7	(3, 1, 3)	1
3	19	(7, 3, 2, 7)	2
4	53	(15, 7, 15, 1, 15)	4
5	126	(31, 15, 31, 3, 15, 31)	6
6	321	(63, 31, 63, 7, 63, 31, 63)	1
7	696	(127, 63, 127, 15, 127, 47, 63, 127)	2
8	1591	(255, 127, 255, 31, 255, 31, 255, 127, 255)	3
9	3446	(511, 255, 511, 63, 511, 255, 63, 511, 255, 511)	2
10	7861	(1023, 511, 1023, 127, 1023, 511, 1023, 63, 1023, 511, 1023)	2
11	≥ 16500	(2047, 1023, 2047, 255, 2047, 1023, 2047, 127, 2047, 1023, 767, 2047)	6*
12	≥ 36083	(4095, 2047, 4095, 511, 4095, 2047, 4095, 255, 4095, 2047, 4095, 511, 4095)	10*
13	≥ 76274	(8191, 4095, 8191, 1023, 8191, 4095, 8191, 511, 8191, 4095, 8191, 1023, 4095, 8191)	14*
14	≥ 168945	(16383, 8191, 16383, 2047, 16383, 8191, 16383, 1023, 16383, 8191, 16383, 2047, 16383, 8191, 16383)	1*

Table 1: Values for $S(n)$ up to dimension $n = 14$.

The alternating 0's mean that there is no solution modeled on a 2-color n-cube with two or more corner types. In addition, minimal n-cubes need 2^n n-cubes of one corner type to construct.

For the right inequality, we will suppose that we have a puzzle $\mathcal{P}$ of the form $(a_0, a_1, \ldots, a_n)$ with no solutions and then bound the sum of the a_i. No a_i can be 2^n or larger, since then a minimal 2-color n-cube could be modeled. Thus $a_i \leq 2^n - 1$ for all $i = 0, \ldots, n$. Additionally, $\mathcal{P}$ does not model a solution of the form $\langle j|1|n-j-1\rangle$ for any $j = 0, \ldots, n-1$. Such 2-color n-cubes are in row 1 of the corner poset and thus have exactly two corner types, coming from two neighboring minimal n-cubes in the bottom row both with multiplicity 2^{n-1}. Hence $\min(a_i, a_{i+1}) \leq 2^{n-1} - 1$ for all $i = 0, \ldots, n-1$. But this implies

$$\begin{aligned}
2\sum_{i=0}^{n} a_i &= a_0 + a_n + \sum_{i=0}^{n-1}(a_i + a_{i+1}) \\
&= a_0 + a_n + \sum_{i=0}^{n-1}\left(\max(a_i, a_{i+1}) + \min(a_i, a_{i+1})\right) \\
&\leq 2 \cdot (2^n - 1) + n\left(2^n - 1 + 2^{n-1} - 1\right) \\
&= 2^{n-1} + 3 \cdot 2^{n-1} - 2 + n\left(3 \cdot 2^{n-1} - 2\right) \\
&= (n+1)\left(3 \cdot 2^{n-1} - 2\right) + 2^{n-1},
\end{aligned}$$

so

$$\sum_{i=0}^{n} a_i \leq (n+1)\left(\frac{3}{4}\cdot 2^n - 1\right) + 2^{n-2},$$

as needed. In particular, if a puzzle has size $(n+1)\left(\frac{3}{4}\cdot 2^n - 1\right) + 2^{n-2} + 1$, it must have a solution in one of the bottom two rows of the corner poset. □

Remark 6.6. A quick look at the values in Table 1 (and the proof of Theorem 6.5) suggests that puzzles $\mathcal{P}$ which realize the value of $S(n)$ have a lot of structure. The most important observation is that for n even, every other entry is the maximum possible size, $2^n - 1$. Such regularity is not possible for n odd, but the maximum value of $2^n - 1$ still occurs as much as possible. If this is, as we believe, true in general, then one could conduct a more extensive computer search, which could potentially reveal additional structure in the answer.

Suppose we have an asymptotic of the form $S(n) \sim cn2^n$, that is,

$$\lim_{n\to\infty} \frac{S(n)}{n2^n} = c. \tag{5}$$

Then the inequalities in Theorem 6.5 imply $0.5 \leq c \leq 0.75$. We can improve on the lower bound here.

Proposition 6.7. *Assume Equation* (5) *holds for some constant c. Then*

$$c \geq \sum_{k=0}^{\infty} 2^{-k-2^k} = 0.64111423493....$$

Proof. We will show how one can construct large puzzles without solutions by exploiting the "upside-down" Pascal property of the corner poset, which we will now describe. As in Section 6, each 2-color n-cube in the poset can be regarded as an $n+1$-tuple corner set $[b_0, b_1, \ldots, b_n]$ where b_i denotes the number of corners of type i corresponding to the corner type of the minimal 2-color n-cube $\langle i|0|n-i\rangle$. By Equation (2), the n-cube $\langle j|k|n-j-k\rangle$ has exactly

$$2^{n-k}\binom{k}{\ell} \tag{6}$$

corners of type $j+\ell$ for $0 \leq \ell \leq k$. The "upside-down" property seen in Equation (7) implies that if a puzzle fails to have a solution modeled on two adjacent n-cubes in the poset, $H_1 = \langle j|k|n-j-k\rangle$ and $H_2 = \langle j+1|k|n-(j+1)-k\rangle$, because there are not enough corners of a particular type, then there is no solution modeled on the n-cube above them, $H_3 = \langle j|k+1|n-j-(k-1)\rangle$ either. This follows from the observation that the number of corners of type m in H_3 is the average of the number of corners of type m in H_1 and H_2. In particular, fix a corner m, and use Equation (6) to count these corners in H_1, H_2, and H_3. One confirms that

$$\frac{1}{2}\cdot 2^{n-k}\left(\binom{k}{m-j} + \binom{k}{m-(j+1)}\right) = 2^{n-(k+1)}\binom{k+1}{m-j} \tag{7}$$

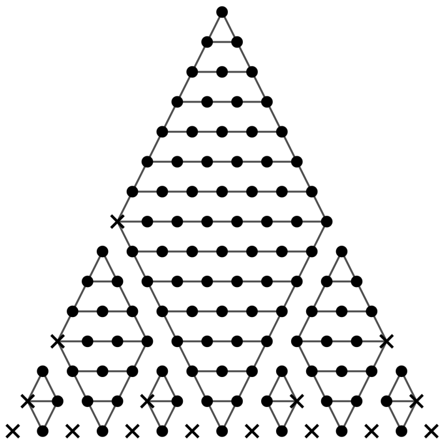


Figure 7: Construction for Proposition 6.7 in dimension 14.

where the binomial coefficient is 0 when the bottom number is negative.

Let n be an integer of the form 2^i-2. Posets of this type can be covered by rhombi as in Figure 7, where a rhombus may consist of a single entry in the poset. Note that every entry on the bottom row belongs to a unique rhombus. Let $k(m)$ denote the row index of the $\times$ in the rhombus containing the minimal cube $\langle m|0|n-m\rangle$ with corner type m. Recall that we denote the bottom of the corner poset as row 0 and index up. Here $k(m)$ is always one less than a power of 2. We claim that if we take $a_m = 2^{n-k(m)}-1$, then the corresponding puzzle $\mathcal{P} = (a_0, a_1, \ldots, a_n)$, has no solution.

It is clear that n-cubes corresponding to $\times$'s in row 0 cannot be built from 2^n-1 cubes of the same type. For larger rhombi, we note that for n-cubes on the lower left and lower right edges of the rhombus require $2^{n-k(m)}$ or more corners of type m for their construction by Equation (6), but $\mathcal{P}$ only contains $2^{n-k(m)}-1$ minimal cubes with this corner type. Now, since there are insufficient minimal cubes with corner type m to construct both n-cubes in row 1 in the rhombus, by Equation (7) there are not enough to construct the n-cubes in row 2 in the rhombus. Continued application of Equation (7) shows that there are not enough minimal cubes with corner m to construct any n-cube in the rhombus. Since the rhombi cover the poset, $\mathcal{P}$ has no solution.

The puzzles we have constructed have the form

$$\begin{aligned}&(2^n-1, 2^{n-1}-1, 2^n-1, 2^{n-3}-1, 2^n-1, 2^{n-1}-1, 2^n-1, 2^{n-7}-1,\\ &\ 2^n-1, 2^{n-1}-1, 2^n-1, 2^{n-3}-1, 2^n-1, 2^{n-1}-1, 2^n-1, 2^{n-15}-1, \ldots).\end{aligned}$$

This construction leads to the inequality

$$\begin{aligned}\lim_{n\to\infty}\frac{S(n)}{n2^n} &\geq \lim_{n\to\infty}\left(\frac{1}{n}+\frac{1}{2n}+\frac{1}{n}+\frac{1}{2^3n}+\frac{1}{n}+\frac{1}{2n}+\frac{1}{n}+\frac{1}{2^7n}+\cdots\right)\\ &= \lim_{n\to\infty}\left(\frac{n}{2}\cdot\frac{1}{n}+\frac{n}{4}\cdot\frac{1}{2n}+\frac{n}{8}\cdot\frac{1}{2^3n}+\frac{n}{16}\cdot\frac{1}{2^7n}+\cdots\right)\end{aligned}$$

$$= \frac{1}{2^1 \cdot 2^{2^0-1}} + \frac{1}{2^2 \cdot 2^{2^1-1}} + \frac{1}{2^3 \cdot 2^{2^2-1}} + \frac{1}{2^4 \cdot 2^{2^3-1}} + \cdots$$
$$= \frac{1}{2^{2^0+0}} + \frac{1}{2^{2^1+1}} + \frac{1}{2^{2^2+2}} + \frac{1}{2^{2^3+3}} + \cdots$$

as claimed. □

We remark that $T(n) = 1$ in Table 1 when $n = 2^i - 2$, $i = 2, 3, 4$, reinforcing the special structure of cases of this form. In future work, we would like to determine the exact value of c. Interestingly, this lower bound 0.64111423493... appears in an analysis of the performance of a family of divide and conquer algorithms for computing the Walsh-Hadamard transform, used in signal/image processing [12].

We provide a couple of generalizations to the puzzle presented in this paper and an additional problem for future exploration.

1. One can restrict puzzles to n-cubes which have a proper 2-coloring, that is, where both black and white facets occur. This leaves out only two n-cubes, the monochrome ones. Lemma 6.4 will still hold, but the types of minimal 2-color n-cubes will change. In particular, the $\langle 0|0|n \rangle$ and $\langle n|0|0 \rangle$ cubes should be replaced with $\langle 0|1|n-1 \rangle$ and $\langle n-1|1|0 \rangle$ cubes. This will clearly change the values in Table 1, although we expect that Theorem 6.5 will still be valid.

2. This article is concerned with the analysis of the 2-color version of the cube stacking puzzle. Variations of the puzzle can be constructed for any number of colors. Considering prior work, such as [2] and [4], we expect this analysis to be challenging.

3. In the discussion before Theorem 6.5, we noted that the constraints on the optimization form an expression that can be converted to conjunctive normal form, suggesting that this optimization problem might be hard. However, the form of the puzzles in Table 1 provide some evidence that a polynomial time algorithm to determine the value of $S(n)$ might exist. What more can be said about the nature of the algorithm?

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