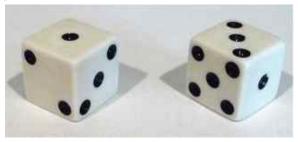
MOVING FACES TO OTHER PLACES: FACET DERANGEMENTS

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ABSTRACT. Derangements are a popular topic in combinatorics classes. We study a generalization to face derangements of the n-dimensional hypercube. These derangements can be classified as odd or even, depending on whether the underlying isometry is direct or indirect, providing a link to abstract algebra. We emphasize the interplay between the geometry, algebra and combinatorics of these sequences, with lots of pretty pictures.

1. Introduction

Suppose you have a die sitting on a table. Instead of just looking at the number on the top of the die, pay attention to the location of the numbers on all six sides. Now you pick it up and roll it so that it occupies the same place on the table it did before. How many ways could you have done this so that none of the 6 numbers are in the same place?



Rolling a die so that it occupies the same place it did before it was rolled gives a *direct isometry* of the cube, i.e., a geometric transformation realizable in 3 dimensions that fixes the cube. Then our question becomes:

How many direct isometries of the cube are *derangements* of the faces of the cube?

How many additional derangements do you get if you allow yourself to turn your cube inside out (allowing an indirect isometry via a roll through 4-dimensional space)? Generalizing, if you have an *n*-dimensional hypercube, then the same question makes sense, although it's a bit harder to buy one and actually roll it.

We'll need a few important facts about isometries in n dimensions. Every isometry can be written as a composition of reflections through hyperplanes. An isometry is direct if it can be written as a composition of an even number of reflections, otherwise, it is indirect (as with products of transpositions in symmetric groups, this

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is well-defined). Further, a direct isometry is orientation preserving, while an indirect isometry reverses orientation. The composition of two reflections is a rotation, provided the hyperplanes corresponding to those reflections intersect. This will always be the case with the isometries we consider here since we will be considering isometries of regular solids whose centers will always be fixed.

The total number of isometries of an n-cube is $2^n n!$ – see Chapters 5 and 7 of Coxeter's classic [7] for a guide to understanding the geometry of these isometries. Half of these are direct and half are indirect.

We now have several questions at hand:

- How many of the $2^n n!$ isometries are derangements of the (n-1)-dimensional faces (also called facets) of the n-cube?
- How many of these facet derangements are direct and how many are indirect?
- What if our die is not a cube (or hypercube)? In particular, what are the counts for a die shaped as an *n*-dimensional simplex?

The answers will lead us to integer sequences that have been studied before in several contexts, as well as to two new sequences. In particular, the sequences associated with the direct and indirect facet-derangements of the n-cube do not appear in Sloane's Online Encyclopedia of Integer Sequences (OEIS, [12]).

These problems lie at the intersection of three fields: combinatorics, geometry and algebra. Our philosophy is mathematically inclusive here. Derangements are typically studied in combinatorics classes, where they provide a good example of inclusion-exclusion. Students need to take a class in abstract algebra to see even and odd permutations. Finally, isometries of Euclidean space might appear in a geometry class emphasizing transformations. But no one class typically presents all three topics coherently.

Derangements of faces of different dimensions of the cube have been studied before. In [4], Chen and Stanley derive explicit generating functions that count derangements of the vertices, edges and 2-dimensional faces for an n-cube; the number of isometries that do fix at least one vertex is given by an especially attractive formula: $(2n-1)!! = (2n-1)(2n-3)\cdots 3\cdot 1$. Chen and Zhang study the excedance of a signed permutation in [3] and [6], and Chen, Tang and Zhao [5] generalize this approach to derangement polynomials. In a different direction, Shareshian and Wachs give an interesting connection to combinatorial topology in [11], where Theorem 6.2 shows that the number of facet derangements of the n-cube is the dimension of the reduced homology of the order complex of a certain poset.

Most of the material we present here is known, but our approach seeks to unify the combinatorics, algebra and geometry. This paper is organized as follows: In Section 2, we begin with a treatment of ordinary derangements from combinatorial, geometric and algebraic viewpoints. Section 3 generalizes the entire approach from Section 2 to the hypercube. This gives us a 'new' combinatorics problem (we call it the *coatcheck problem*, generalizing the hatcheck problem for ordinary derangements), and (what we believe to be) a new recursion for the facet derangements for the n-cube. We also present several known formulas for the number of facet derangements, with proofs that use ideas from combinatorics (inclusion-exclusion) and linear algebra (signed permutation matrices).

Section 4 studies the partition of the facet derangements of the (n-1)-simplex and the n-cube into direct and indirect isometries. This is where the connections to geometry are deepest, and where some very pretty relations are developed.

The geometry of 3 dimensions gives us a chance to test our geometric intuition, so Section 5 describes these isometries and derangements in some detail. We conclude by offering a few suggestions for further study in Section 6.

2. Derangements and simplices

2.1. Counting ordinary derangements. One of the standard problems in a combinatorics class asks the following question:

Hatcheck problem: *n* people check their hats at the beginning of a party. How many ways can the hats be returned later so that no one gets their own hat back?

Slightly more modern versions might involve returning cell phones to students after an exam, or designing a cryptoquote so that no letter stands for itself (usually called a *substitution cypher*) in the coded message.

Permutations of $\{1, 2, ..., n\}$ with no fixed points are called *derangements*. The following formula counting derangments can be found in every combinatorics book in the section that introduces *inclusion-exclusion* as a counting technique. If d_n denotes the number of derangements on an n-element set, then

(1)
$$d_n = n! \sum_{k=0}^n \frac{(-1)^k}{k!}$$

From the formula, we get $d_0 = 1$. You can give any explanation you like for what happens when no people check their hats, as long as you get the answer 1.

This formula has a very attractive probabilistic consequence: If the hats are randomly returned to the party-goers, then the probability that no one receives their own hat is approximately $e^{-1} \sim 36.79\%$. When n is large, this probability is (essentially) independent of n, which is surprising (unless you already know this, in which case it isn't). The number of derangements for $n \leq 7$ is given in Table 1. Note that the ratio $d_7/7!$ agrees with $e^{-1} \approx 0.367879\ldots$ to 4 decimals.

Table 1. Number of derangements d_n for $n \leq 7$.

n	0	1	2	3	4	5	6	7
d_n	1	0	1	2	9	44	265	1854
$\frac{d_n}{n!}$	1	0	0.5	$0.\bar{3}$	0.375	$0.3\bar{6}$	$0.3680\bar{5}$	0.367857

We end this preliminary discussion with one more formula – a very useful recursion for d_n that we'll refer to later:

(2)
$$d_n = (n-1)(d_{n-1} + d_{n-2})$$

The proof of this recursion follows from partitioning the derangements into those in which 1 participates in a 2-cycle and those in which 1 is in a longer cycle. A proof can be found in [1], for instance.

2.2. **Derangements and the** (n-1)-simplex. Our first goal is to interpret derangements geometrically, as derangements of the facets (or vertices) of the (n-1)-simplex. Recall the (n-1)-simplex is formed by joining n affinely independent points in \mathbb{R}^{n-1} , so the 2-simplex is a triangle in the plane, the 3-simplex is a tetrahedron in 3-space, and so on.

Geometric Interpretation: A derangement on $\{1, 2, ..., n\}$ corresponds to an isometry in \mathbb{R}^{n-1} of the regular (n-1)-simplex in which every one of the n facets is moved.

Why does this work? First, the full symmetry group (including both direct and indirect isometries) of the regular (n-1)-simplex is the symmetric group S_n . The group is usually thought of as acting on the n vertices of the simplex, but since every facet has a unique vertex it does not touch, a permutation moves a vertex if and only if it moves the 'opposing' facet. Thus, for our purposes, we will think of S_n as acting on the facets of the (n-1)-simplex.

In 2 dimensions, a simplex is an equilateral triangle in the plane. There are only two kinds of isometries possible: rotations (direct) and reflections (indirect). This group of isometries is easy to visualize via the six edge permutations of the triangle. The correspondence between the isometries and the permutations is given in Fig. 1.

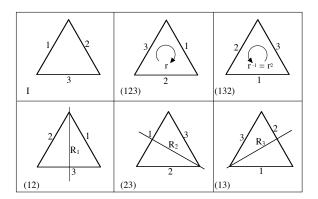


FIGURE 1. Symmetry group $= S_3 \cong D_3$

Which of these are derangements? The two rotations r = (123) and $r^2 = (132)$ derange the edges, and the remaining four permutations fix at least one edge, so $d_3 = 2$, as we saw earlier.

In 3 dimensions, we need to add one more isometry to our tool kit: rotary reflections. These can be hard to visualize - they correspond to compositions of reflections and rotations. For some fun (and a good exercise in geometric visualization), try to figure out the geometry of the facet derangements in 3 dimensions. You should get the following:

• For the regular tetrahedron, there are 9 derangements: 3 of these are rotations and the remaining 6 are rotary reflections.

Much more information about the geometry of isometries in 3 dimensions – and some very attractive pictures – appears in Section 5. Feel free to skip ahead.

3. Deranging the facets of a hypercube

3.1. A problem with coats and cubes. In Section 2, we saw that ordinary derangements correspond to isometries of a regular (n-1)-simplex in which no (n-1)-dimensional facet is fixed. To generalize this to facet derangements of hypercubes, we need to modify the hatcheck problem:

Couples coatcheck problem This time, *n couples* each check their two coats at the beginning of a party; the attendant puts a couple's coats on a single hanger. The coats are returned at the end of the party in the following way: when a couple arrives to get their coats, the (lazy) attendant picks an arbitrary hanger and then hands one of those coats to one person in the couple and the other coat to the other (again, arbitrarily). How many ways can the coats be returned so that no one gets their own coat back?

If no one receives their own coat, we'll say we have a *c-derangement* (where 'c' stands for 'coat' or 'couple' or 'cube'). Evidently, there are two ways the people in a couple could fail to receive their own coats: Either the pair of coats belonging to that couple was given to another couple, or the couple did receive their own coats, but the coats were swapped between the two partners.

As before, we begin by interpreting this combinatorial problem geometrically.

Geometric Interpretation: A c-derangement corresponds to an isometry in \mathbb{R}^n of the hypercube in which no (n-1)-dimensional facet is fixed.

Why is this true? First, note that there are $2^n n!$ ways to return the coats with no restrictions:

- First, permute the n hangers in n! ways;
- Next, hand the coats back to the two members of each couple in 2^n ways.

But this is precisely the number of isometries of the n-dimensional hypercube:

- First, permute the n facets around a given vertex in n! ways;
- Next, swap or don't swap each pair of opposite facets in 2^n ways.

Let's introduce some notation: Let Q_n denote the regular n-dimensional hypercube. The 2n people are represented by the 2n symbols $1, 1^*, 2, 2^*, \ldots, n, n^*$, where $\{i, i^*\}$ is the i^{th} couple. Then the 2n facets of Q_n correspond precisely to the 2n people in the coatcheck problem, with the couple $\{i, i^*\}$ corresponding to that pair of opposite facets in the hypercube. It should now be clear that moving all the facets of Q_n is equivalent to deranging the coats. (Unlike the connection between ordinary derangements and the simplex, deranging vertices is not the same as deranging facets. In Figure 2, you can locate a c-derangement of the square that is not a vertex derangement, and then find a vertex-derangement that's not a c-derangement.)

A 2-dimensional cube is a square, and its facets are the 4 bounding edges. Among the 8 symmetries of a square (which form the dihedral symmetry group D_4), there are 5 c-derangements, pictured in Figure 2. The original square is in the upper left. The other two squares in the top row arise from reflections through the diagonals of the square, and the 3 squares in the bottom row of the figure arise from rotations.

As with the simplex, the geometry is fun to explore in 3 dimensions. We return to this (in great detail) in Section 5. For now, though, see if you can determine

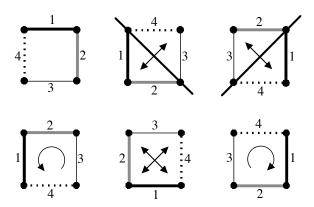


FIGURE 2. The 5 side-derangements of the square.

which isometries of the cube are derangements. As a check, you should get the following:

- For the cube, there are 29 derangements: 14 rotations and 15 rotary reflections
- 3.2. Some formulas for c-derangements. We are ready to derive some formulas for the number of c-derangements. Let \hat{d}_n be the number of c-derangements of $\{1, 1^*, \ldots, n, n^*\}$. As in the ordinary derangement case, we can find a formula for \hat{d}_n using inclusion-exclusion. This formula is listed for sequence A000354 in the OEIS [12], but the interpretation in terms of c-derangements is not mentioned there.

Theorem 3.1. The number \hat{d}_n of c-derangements of the facets of Q_n is given by

(3)
$$\hat{d}_n = \sum_{k=0}^n (-1)^k \binom{n}{k} 2^{n-k} (n-k)!$$

Proof. First, place the *n*-dimensional hypercube so that one vertex is at the origin and the opposite vertex is at the point $(1,1,\ldots,1)$. Then Q_n has n facets with one vertex at the origin, and we need only consider what happens to those facets to determine what happens to all the facets of Q_n .

We use inclusion-exclusion. The number of c-derangements will be the total number of isometries of Q_n , minus the number that fix at least one facet, plus the number that fix at least 2 facets, etc.

The number of isometries of Q_n that fix at least 0 facets is just the total number of isometries of Q_n , that is, $2^n n!$. To fix k (or more) facets, we choose those k in $\binom{n}{k}$ ways, and then consider the number of automorphisms of the rest, which is $2^{n-k}(n-k)!$. This gives the formula.

Note that a consequence of this formula is that $d_0 = 1$. Again, you can figure out what that means yourself. Also notice that this formula guarantees that \hat{d}_n is always odd: every term in Equation 3 is even except for the term corresponding to k = n. We'll see two more proofs of this fact later – pay attention.

As with ordinary derangements, we can use this result to get a nice probabilistic interpretation. Rewriting the above formula as

(4)
$$\hat{d}_n = 2^n n! \sum_{k=0}^n (-1/2)^k \frac{1}{k!}$$

gives us the following:

In the coatcheck problem, the probability that no one receives their own coat approaches $e^{-1/2}$ as the number of couples increases.

Table 2 gives the number of c-derangements for $n \leq 7$. When n = 6, the approximation to $e^{-1/2} \approx 0.606531...$ is accurate to 5 decimals. This series converges faster than the series for e^{-1} that gave the number of (ordinary) derangements, as you would expect from the Taylor series error estimate.

2 3 1 1 5 d_n 29 d_n 1 0.50.6250.6041... $\overline{2}^n n!$ 7 6 5 233 2329 27,949 391,285 d_n d_n 0.606770...0.606510...0.606532...0.606530... $\overline{2^n n!}$

Table 2. Number of c-derangements $\hat{d_n}$ for $n \leq 7$.

There is another formulation for d_n that we like. We can express d_n with a sum that uses the ordinary derangements d_k . The proof uses signed permutation matrices, which will be important for us in Section 4 when we consider the orientation of a c-derangement, i.e., whether the c-derangement corresponds to a direct or an indirect isometry of the hypercube.

Proposition 3.2. The number of c-derangements of the facets of Q_n is

$$\hat{d_n} = \sum_{k=0}^n \binom{n}{k} 2^k d_k.$$

Proof. Situate Q_n so that all its vertices are located at the points $(\pm 1, \pm 1, \ldots, \pm 1)$. Then the centers of the facets are $\pm e_i$, where e_i is the i^{th} standard basis vector in \mathbb{R}^n . Now any isometry of Q_n sends the facet corresponding to e_i to another facet $\pm e_j$. Thus, an isometry can be identified with a *signed permutation matrix*, a permutation matrix with with entries ± 1 . (There are clearly $2^n \cdot n!$ such matrices.)

Now let A be a signed permutation matrix that corresponds to a facet derangement. Then there are no 1's on the main diagonal of A. (An entry of -1 along the main diagonal corresponds to sending a facet to its opposite.) It remains to count the number of such matrices.

Suppose A has k 0's along its main diagonal. Then the remaining n-k diagonal entries must be -1's. We can view the action of A on Q_n as follows: A fixes the n-k facet pairs corresponding to the -1's on the diagonal (swapping the facets

within each such pair), and A deranges the remaining k facet pairs. We can choose the k facet pairs to derange in $\binom{n}{k}$ ways, then derange those pairs in d_k ways. But there are two choices for each such pair: If the pair $\{e_i, -e_i\}$ is sent to $\{e_j, -e_j\}$, then either $e_i \mapsto e_j$ (and so $-e_i \mapsto -e_j$), or $e_i \mapsto -e_j$ (so $-e_i \mapsto e_j$).

Thus, the total number of c-derangement signed permutation matrices having k 0's on their diagonals is just $\binom{n}{k} 2^k d_k$. The formula follows by summing over k.

One way to visualize the derivation of Equation (5) is suggested by Figure 3. In the figure, assume that two pairs of opposite facets of a 5-dimensional cube are interchanged, so $i \leftrightarrow i^*$ and $j \leftrightarrow j^*$, corresponding to two -1's on the main diagonal of the signed permutation matrix. Then the two facet pairs (i, i^*) and (j, j^*) are 'shrunk,' leaving a 3-cube. That cube will then have its pairs of opposite faces deranged in d_3 ways (since we don't allow opposite faces to be interchanged), and then pairs of opposite sides can be oriented in 2^3 ways.

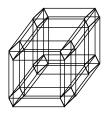


FIGURE 3. A 5-cube with two sets of opposite facets that will be interchanged; the remaining 3 pairs will be deranged.

A generalization of Equation (5) appears in [13], where Spivey and Steil define the rising k-binomial transform of a sequence a_n to be

$$r_n = \begin{cases} \sum_{i=0}^n \binom{n}{i} k^i a_i & \text{if } k \neq 0 \\ a_0 & \text{if } k = 0. \end{cases}$$

Then the sequence \hat{d}_n is the rising 2-binomial transform of the sequence d_k . The explicit connection to c-derangements does not appear in that paper, however.

The following recursion generalizes the recursion for ordinary derangements given in Equation (2). The recursion appears to be new. It also gives an inductive proof that \hat{d}_n is always odd (our second proof of this fact).

Proposition 3.3. For n > 2, $\hat{d_n}$ satisfies:

(6)
$$\hat{d}_n = (2n-1)\hat{d}_{n-1} + (2n-2)\hat{d}_{n-2}$$

Proof. This proof is modeled on the proof of Equation (2). That proof partitions derangements into 2 classes: those in which 1 is interchanged with some k > 1 and those in which 1 is in a cycle of length greater than 2. For c-deragements, we have an additional case arising from the fact that a pair (i, i^*) can be fixed but swapped and additional complications because there are multiple ways to send (i, i^*) to (j, j^*) .

There are three cases to consider for c-derangements.

Case 1: The pair $(1,1^*)$ is fixed by the c-derangement. In this case, 1 and 1^* must be swapped and the remaining n-1 pairs are c-deranged. This gives a total of \hat{d}_{n-1} c-derangements. (This case does not appear in the proof of the ordinary derangement recursion (2).)

Case 2: The pair $(1,1^*)$ is swapped with some other pair (k,k^*) . There are n-1 choices for the (k,k^*) pair, and then there are 4 ways to swap the pairs $(1,1^*)$ and (k,k^*) : (1) 1 \leftrightarrow k, 1* \leftrightarrow k^* ; or (2) 1 \leftrightarrow k^* , 1* \leftrightarrow k; or (3) 1 \to $k \to 1^* \to k^* \to 1$; or (4) 1 \to $k^* \to 1^* \to k \to 1$.

The remaining n-2 pairs can be c-deranged in \hat{d}_{n-2} ways. This gives a total of $4(n-1)\hat{d}_{n-2}$ c-derangements.

Case 3: 1 is in a cycle of length greater than 2. If $(1,1^*) \to (k,k^*)$, then by assumption, $k \neq 1$ and $(k,k^*) \not\mapsto (1,1^*)$. There are n-1 choices for k, and there are 2 ways to send $(1,1^*)$ to (k,k^*) . Since $(k,k^*) \mapsto (i,i^*)$, where $(i,i^*) \neq (1,1^*)$, we can simply replace (k,k^*) by either $(1,1^*)$ or $(1^*,1)$, depending on how $(1,1^*)$ mapped to (k,k^*) in the original c-derangement. This gives us a c-derangement on n-1 pairs with the additional restriction that the pair $(1,1^*)$ is not mapped to itself. (This restriction is a consequence of the fact that we can't send (k,k^*) to $(1,1^*)$.)

How many of the \hat{d}_{n-1} derangements require that $(1,1^*)$ not be sent to itself? The number of c-derangements of n-1 pairs in which one pair is sent to itself is \hat{d}_{n-2} (this is just Case 1 for the remaining n-1 pairs). Thus, the final total in this case is $2(n-1)(\hat{d}_{n-1}-\hat{d}_{n-2})$ derangements.

These three cases give that $\hat{d}_n = \hat{d}_{n-1} + 4(n-1)\hat{d}_{n-2} + 2(n-1)(\hat{d}_{n-1} - \hat{d}_{n-2}) = (2n-1)\hat{d}_{n-1} + (2n-2)\hat{d}_{n-2}$, as desired.

Notice that \hat{d}_2 and the values you get from the recursion depend on the (somewhat disturbing) fact that $\hat{d}_0 = 1$.

4. The parity of derangements and c-derangements

4.1. Counting direct and indirect (ordinary) derangements. As we've seen, isometries can be either direct or indirect, depending on whether they can be expressed as a product of an even or odd number of reflections, resp. The direct isometries of a simplex correspond to even permutations of $\{1, 2, ..., n\}$, and the indirect ones correspond to odd permutations.

For the facet derangements of a simplex, here's what we have seen so far: For the triangle, both derangements are rotations, and so are direct isometries. For the regular tetrahedron, there are 9 derangements: 3 rotations (direct) and 6 rotary reflections (indirect). See Section 5 for a full explanation for the tetrahedron.

We let e_n denote the number of direct derangements of the facets of an (n-1)-simplex and o_n denote the number of indirect derangements. Table 3 gives the values of d_n , e_n and o_n for $n \le 7$.

A very casual glance at the last row of the table should suggest a very pretty theorem. This pattern is not new; for example, you can find the sequences e_n and o_n in the OEIS [12]. A bijective proof using a conjugation argument can be found in [2], and the recent paper [9] offers two more proofs based on an analysis of

n	1	2	3	4	5	6	7
d_n	0	1	2	9	44	265	1854
e_n	0	0	2	3	24	130	930
o_n	0	1	0	6	20	135	924
$e_n - o_n$	0	-1	2	-3	4	-5	6

Table 3. Number of even and odd derangements for $n \leq 7$.

excedances of permutations. The proof we give is inductive and more in line with what we have done to this point.

Theorem 4.1. Let e_n and o_n be the respective number of even and odd derangements of $\{1, 2, ..., n\}$. Then $e_n - o_n = (-1)^{n-1}(n-1)$.

Proof. We give a recursive procedure for computing e_n and o_n . The proof then follows by induction. The key observation is the familiar recursion given in Equation (2): $d_n = (n-1)(d_{n-1} + d_{n-2})$.

Adapting this recursion to include the parity of the derangements is easy: If 1 is in a transposition, we just remove that transposition. If 1 is not in a transposition, then we just remove 1 from the cycle it participates in. In either case, this process changes even permutations to odd ones, and vice versa.

We let e'_n denote the even derangements in which the transposition (1r) appears for some r > 1 and e''_n denote the other even derangements, and define o'_n and o''_n similarly. Then $e_n = e'_n + e''_n$ and $o_n = o'_n + o''_n$. This gives the following recursive relations:

$$e'_n = (n-1)o_{n-2}$$
 $e''_n = (n-1)o_{n-1}$ $o'_n = (n-1)e_{n-2}$ $o''_n = (n-1)e_{n-1}$
Then

$$e_{n} - o_{n} = (e'_{n} + e''_{n}) - (o'_{n} + o''_{n})$$

$$= (n-1)((o_{n-1} + o_{n-2}) - (e_{n-1} + e_{n-2}))$$

$$= (n-1)((o_{n-1} - e_{n-1}) + (o_{n-2} - e_{n-2}))$$

$$= (n-1)((-1)^{n-1}(n-2) + (-1)^{n-2}(n-3))$$

$$= (-1)^{n-1}(n-1).$$

The formula now follows by induction, using the initial values from Table 3.

Corollary 4.2. Let e_n and o_n be the number of even and odd derangements, resp. Then $e_n = \frac{d_n + (-1)^{n-1}(n-1)}{2}$ and $o_n = \frac{d_n + (-1)^n(n-1)}{2}$.

We don't believe Theorem 4.1 is as well-known as it should be. As we remarked earlier, we believe this has to do with the fact that students study derangements in combinatorics classes, but they study permutation groups in algebra classes.

4.2. Counting direct and indirect c-derangements. How can we determine whether an isometry of Q_n is direct or indirect? We know that direct isometries are the product of an even number of reflections, but in this setting, it can be confusing to interpret reflections using permutation notation. For instance, consider the following c-derangement of the cube in 3-dimensions:

- First, reflect in a plane that contains two edges of the cube to get the facet permutation $(1,2)(1^*,2^*)$.
- Then reflect in a plane parallel to facets 3 and 3^* : $(3,3^*)$.

The result is a c-derangement whose facet cycle structure is $(1,2)(1^*,2^*)(3,3^*)$. This *looks* like a product of an odd number of transpositions, but this isometry is *direct* (and so, in this case, it's a rotation). The problem with our algebraic representations of the isometries is the redundancy in representing the reflection $(1,2)(1^*,2^*)$.

We can work around this problem by finding a more concise way to represent an isometry. For our example, the representation of the first isometry has the following redundancy: If facets 1 and 2 are swapped, then the isometry also must swap 1* and 2*. Thus, we can recode the isometry as follows: $(1,2)(3,3^*)$. Similarly, we can recode $(1,2^*)(1^*,2)$ as $(1,2^*)$ (of course, we could also recode it as $(1^*,2)$ if we wanted).

For readers who know more group theory, this recoding can be made precise by using the group of isometries of the hypercube, called the *hypercotahedral* group (it's the same as the isometry group of the dual solid - the *hypercotahedron* or the *n*-dimensional cross-polytope [7]). This group is isomorphic to $\mathbb{Z}_2^n \rtimes S_n$, the semidirect product of the normal abelian 2-group \mathbb{Z}_2^n and the symmetric group S_n , where the action of S_n on \mathbb{Z}_2^n is conjugation.

From a geometric perspective, we can think of this group as acting on the facets of the hypercube as follows:

- Situate the hypercube so that the origin $\mathbf{0}$ is one of its vertices and the facets incident to $\mathbf{0}$ are labeled $1, 2, \dots, n$.
- Use elements in S_n to permute the facets surrounding **0**.
- Finally, use reflections in the normal subgroup \mathbb{Z}_2^n to move **0** to some other vertex v.

We saw this procedure earlier in the discussion at the beginning of Section 3 that explained the link between the coat problem and c-derangements. Any permutation in S_n can be written as a product of transpositions, and you can show that interchanging two facets adjacent to $\mathbf{0}$ can be realized as a single reflection. Then the first factor \mathbb{Z}_2^n is generated by n orthogonal reflections normal to the n coordinate axes, and S_n is generated by reflections corresponding to transpositions. More information about this action can be found in [8], for example.

We can now use this to get the 'right' way to represent an isometry of the cube as a product of transpositions. Our goal is to write any isometry of the cube as a product of terms like (i,i^*) followed by terms of the form (i,j). (We use the convention that multiplication is done right to left.) For example, the rotation $(12)(1^*2^*)(33^*)$ would be expressed more simply as $(33^*)(12)$ (since if 1 and 2 are switched, then 1^* and 2^* must also be switched). More complicated but still doable, $(1,2^*)(1^*,2)=(1,1^*)(2,2^*)(1,2)(1^*,2^*)$ which becomes $(1,1^*)(2,2^*)(1,2)$ in our shorthand notation.

Using this representation for the group, we see that an isometry is direct if and only if it is a product of an even number of transpositions (written in the shorthand way), which is what we were after.

An even better way to deal with the direct-indirect issue here is to use the signed permutation matrices we used in the proof of Prop. 3.2. Then we can tell whether an isometry is direct or indirect by evaluating its determinant:

If A is a signed permutation matrix, then det(A) = 1 precisely when A corresponds to a direct isometry, and det(A) = -1 if A corresponds to an indirect isometry.

Reflection	Transposition	Matrix operation
Normal to coordinate axis	(k, k^*)	Multiply row k by -1
Not normal to coordinate axis	$(ab)(a^*b^*)$	Swap rows a and b
Not normal to coordinate axis	$(ab^*)(a^*b)$	Swap rows a and b
		and multiply each by -1

In Section 3 we gave the number of direct and indirect c-derangements for the square and cube. Here's what we asserted:

- Square: $\hat{d}_2 = 5$, with 3 direct and 2 indirect c-derangements.
- Cube: $\hat{d}_3 = 29$, with 14 direct and 15 indirect c-derangements.

The next theorem shows that the difference between the number of direct and indirect c-derangements is always ± 1 . This will follow from the construction of a bijection between the odd and even c-derangements except for central inversion. Central inversion is the isometry that sends every point (x_1, \ldots, x_n) to its antipodal point $(-x_1, \ldots, -x_n)$. For the square, you can see the central inversion in Figure 2 in the center of the bottom row – a 180° rotation indeed sends every point to its antipode. Thus, in dimension 2, central inversion is a direct isometry. In Section 5, we will see that central inversion in dimension 3 is indirect (chemists call this an improper reflection). This pattern continues: the matrix corresponding to central inversion is $-I_{n\times n}$, i.e., the diagonal matrix with all entries -1. Its determinant is ± 1 , depending on the parity of n, the dimension of our hypercube. Thus, central inversion (which is always a c-derangement) is direct in even dimensions and indirect in odd dimensions.

Theorem 4.3. Let \hat{e}_n and \hat{o}_n denote the number of direct and indirect c-derangements of Q_n resp. Then $\hat{e}_n - \hat{o}_n = (-1)^n$.

Proof. To keep track of which c-derangements are direct and which are indirect, we use signed permutation matrices. We will construct a bijection between the direct and indirect c-derangements that are not central inversion. So, assume A is a signed permutation matrix corresponding to a c-derangement that is not central inversion. A has at least 2 non-zero entries off the main diagonal, so we can find i so that $a_{i,i} = 0$ but $a_{m,m} \neq 0$ for all m < i. Let j be the column corresponding to the non-zero entry in row i, so j is the unique index with $a_{i,j} \neq 0$.

We know that $a_{i,j} = 1$ or -1. For one of those choices, the determinant will be 1 and for the other, the determinant will be -1 (since $a_{i,j}$ is the only non-zero entry in that row, and multiplying a row by -1 multiplies the determinant by -1). Since both choices are c-derangements, this gives us the bijection between the direct and indirect c-derangements (where we have removed central inversion from consideration). Putting central inversion back in gives us the formula, since central inversion is direct if and only if n is even.

Theorem 4.3 gives a third proof¹ that \hat{d}_n is always odd: $\hat{d}_n = 2\hat{e}_n \pm 1$. In Table 4, we list the first 7 values of the sequences \hat{e}_n and \hat{o}_n .

Table 4. Number of even and odd c-derangements for $n \leq 7$.

n	1	2	3	4	5	6	7
\hat{d}_n	1	5	29	233	2329	27,949	391,285
\hat{e}_n	0	3	14	117	1164	13,975	195,642
\hat{o}_n	1	2	15	116	1165	13,974	195,643

Corollary 4.4. Let \hat{e}_n and \hat{o}_n denote the number of direct and indirect c-derangements of Q_n resp. Then $\hat{e}_n = \frac{\hat{d}_n + (-1)^n}{2}$ and $\hat{o}_n = \frac{\hat{d}_n + (-1)^{n+1}}{2}$.

The sequences \hat{e}_n and \hat{o}_n appear to be 'new' in the sense they are not (currently) in the OEIS [12].

5. Geometry of 3-dimensional derangements and c-derangements

Time for some fun. If, like most humans, you have trouble visualizing objects in 4 or more dimensions, then you can start by looking at some low dimensional examples, and then try to generalize. This sounds easier than it is, but, for the simplex and hypercube symmetries, it's extremely valuable. An interesting discussion about the power of analogy appears in Section 7-1 of [7].

5.1. **Derangements of the tetrahedron.** For a bounded solid in \mathbb{R}^3 , there are three kinds of isometries we need to consider: rotations, reflections and *rotary reflections*. Rotary reflections are operations that correspond to combining a rotation and a reflection. It is possible to have a rotary reflection where neither the rotation nor the reflection involved is itself a symmetry of the object; when this happens, the rotary reflection is called *irreducible*.

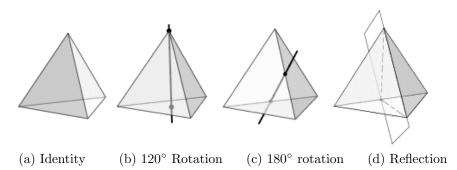


FIGURE 4. A tetrahedron, a 120° rotation, a 180° rotation and a reflection.

The tetrahedron has 24 symmetries corresponding to the 4! permutations of S_4 . As isometries, these can be broken into the following categories.

• Direct isometries

¹Three proofs mean it's really really really true.

- The identity I, which is clearly not a derangement;
- The 8 rotations with axis through a vertex and the center of the opposite facet as in Figure 4(b). These order 3 rotations are through angles of 120° or 240° and correspond to face permutations of the form (abc). These are not derangements;
- \circ The 3 180° rotations with axis through the centers of two opposite edges as in Figure 4(c). They have face permutations (ab)(cd) and so are derangements.

• Indirect isometries

- The 6 reflections with mirror plane containing one edge of the tetrahedron as in Figure 4(d). These have face permutations of the form (ab), so they aren't derangements;
- The 6 rotary reflections, with face permutation form (abcd) as in Figure 5. These are derangements.

It's worth investigating more closely how the rotary reflections operate. The following step-by-step guide should help you create any of the 6 rotary reflections on your own tetrahedron.

- (1) Cut the tetrahedron through the plane containing the centers of four edges (take all edges except two that do not share a vertex). This cuts the tetrahedron into two congruent pieces that get glued back along a square. (You now have a tricky little puzzle.)
- (2) Rotate the entire tetrahedron 90° about an axis perpendicular to the square cross-section. This is *not* an isometry of the tetrahedron.
- (3) Reflect the tetrahedron through the plane containing the square. This is also not an isometry of the tetrahedron.

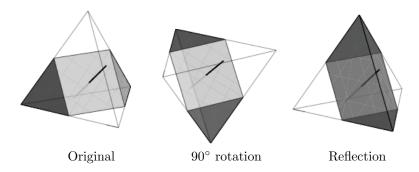


FIGURE 5. A rotary reflection in two steps: First rotate (the tetrahedron does not match up), then reflect.

You didn't really need to cut your tetrahedron into two pieces after all, but you do need to identify the square cross-section. The rotation involved is 'half' of one of our 180° edge-rotations from Figure 4(c). The resulting rotary reflection is irreducible. As mentioned above, this rotary reflection induces the face permutation (abcd), a 4-cycle. This shouldn't be too surprising, as the square from the cross-section meets each of the four faces, and we are rotating around this square.

5.2. **c-derangements of the cube.** Now we turn our attention to the ordinary 3-dimensional cube. There are $2^33! = 48$ isometries of a cube:

• Direct isometries

- The identity, which is not a c-derangement;
- Eight rotations of 120° and 240° through the 4 pairs of opposite vertices as pictured in 6(a). These are c-derangements;
- Six 180° rotations through the centers of opposite edges as pictured in 6(b). These are also c-derangements;
- \circ Nine rotations through the centers of opposite faces. These are not c-derangements.

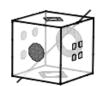
• Indirect isometries

- Nine reflections: three through the plane containing the centers of four parallel edges and six through opposite edges. None of these are c-derangements;
- Fifteen rotary reflections: central inversion (pictured in Figure 7(a)); six reducible ones through an axis through centers of opposite sides (pictured in Figure 7(b)) and eight irreducible ones through an axis through two opposite vertices (pictured in Figure 7(c)). These are c-derangements.

Note that 14 of the 29 c-derangements are direct, while 15 are indirect. In both Figure 6 and Figure 7, opposite facets have the same pattern, but in different sizes. Notice also that the direct isometries preserve the orientation of the cube (so you perform these isometries with a die), while the indirect ones reverse the orientation of the cube (so you'd need a mirror-image die to perform them).









(a) Rotate through opposite vertices

(b) Rotate through opposite edge centers

FIGURE 6. The direct face-derangements of the cube.

The indirect c-derangements are all rotary reflections, which are, again, a bit harder to picture. Central inversion always corresponds to a c-derangement (see Figure 7(a)), but it's an indirect isometry in 3-dimensions. It can be realized either as the composition of 3 mutually perpendicular reflections or by a rotary reflection in a variety of ways, as we will see shortly.

We now examine the 14 remaining rotary reflections in a bit more detail. In Figure 7(b), you can see the rotary reflection formed as a composition of a rotation of 90° or 270° around an axis through the center of two opposite sides followed by a reflection through the plane perpendicular to that axis at its midpoint. There are 3 of those axes so there are 6 such rotary reflections, all of which are reducible. (Notice that if you do this same rotary reflection with a rotation of 180°, you get central inversion).

In Figure 7(c), you can see the last kind of rotary reflection, which is irreducible: a rotation of 60° or 300° around an axis through two opposite vertices followed by a reflection through the plane perpendicular to that axis. Since there are 4 pairs of opposite vertices, this gives 8 distinct isometries. (Once again, central inversion

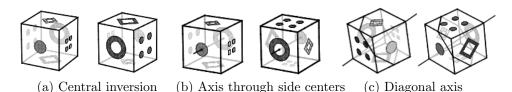


FIGURE 7. The 15 indirect face-derangements of the cube.

arises from a rotation of 180° followed by reflection.) These can be quite challenging to picture, since the initial rotation does not align the cube with itself. Figure 8 breaks an irreducible rotary reflection down to help with visualization.



FIGURE 8. An irreducible rotary reflection of the cube.

There are two more interesting aspects of this kind of rotary reflection. First, it gives a 6-cycle on the faces of the cube. Second, the plane perpendicular to the axis of rotation cuts the cube into two congruent pieces, forming (as a cross section) a regular hexagon that passes through each of the 6 sides of the cube. It is well worth locating these hexagons on an actual cube! Showing students the two pieces (after having them guess about what kinds of polygons could be formed as cross sections when slicing a cube) usually elicits some surprised looks.

6. Suggestions for future study

We conclude with a few ideas for projects that can help solidify some of the ideas from this paper.

- (1) In the proof of Theorem 4.3, signed permutation matrices give a bijection between the direct and indirect isometries (excluding central inversion). As a warm-up, find this bijection explicitly for the 14 direct and 14 indirect (again, excluding central inversion) c-derangements of the cube. (To do this, you will need to number the six faces of your cube 1, 1*, 2, 2*, 3, 3* and then use this numbering to refer to your c-derangements.)
- (2) Study the vertex, edge and face derangements for the remaining Platonic solids. We've covered the faces (and the vertices) for the tetrahedron, and we've done the faces of the cube (and therefore, the vertices of its dual, the octahedron). We haven't considered the faces of the octahedron, and we've completely ignored the icosahedron and its dual, the dodecahedron.

Determining the vertex, edge or facet derangement numbers for these solids is a good exercise in geometric visualization.

The symmetry group of the icosahedron is $A_5 \times \mathbb{Z}_2$, so there are 120 isometries to consider. Counting the direct and indirect vertex, edge and face derangements is also a good exercise. For extra credit, describe the 45 rotary reflections explicitly in this case.

- (3) There are 6 regular solids in 4 dimensions: The 4-simplex, the hypercube the hypercotahedron, the 24-cell, the 120-cell, and the 600-cell. All of the same questions make sense here:
 - Find the number of vertex, edge, 2-dimensional and 3-dimensional face derangement numbers for the 24-cell and the 120-cell. (By duality, derangements for the 120-cell and the 600-cell are the same, where the vertex derangements for the 120-cell are the same as the 3-dimesional facet derangements for the 600-cell, and so on.)
 - For each class of derangements, count the direct and indirect isometries, as above.

The 24-cell has 1152 isometries and the 120-cell (and 600-cell) has 14,400. In dimensions 5 and higher, there are only 3 regular solids: The n-simples, the n-cube its dual, the n-dimensional hyperoctahedron. See [8] for descriptions of these symmetry groups.

(4) Extend this approach to general root systems. In particular, the exceptional root systems E_6 , E_7 and E_8 are very important families of vectors that display lots of symmetry. How many isometries move all the vectors in the root system? Much more about root systems can be found in [8].

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