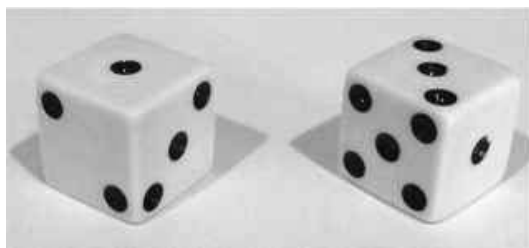

Moving Faces to Other Places: Facet Derangements

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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 locations 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. A *derangement* is a permutation with no fixed points. 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 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 always fix the centers of our solids.

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The total number of isometries of an n -cube is $2^n n!$ —we’ll see why in Section 3.1. Chapters 5 and 7 of Coxeter’s classic [6] offer an excellent guide to understanding the geometry of these isometries. Half 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 are new sequences in Sloane’s Online Encyclopedia of Integer Sequences (OEIS, [11]), arising from this paper.

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 the principle 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 [3] considers the entire cycle structure (encoded by the cycle index polynomial) of the vertices of the hypercube, while the *excedance* of a signed permutation is explored by Mataci and Rakotandrajao in [8]. 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 [10], 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. 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 *couples 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.

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 relationships 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 his or her 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 $\{1, 2, \dots, n\}$ with no fixed points are called *derangements*. The following formula that gives the number of derangements 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

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

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 his or her own hat is approximately e^{-1} . 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 $e^{-1} \approx 0.367879\dots$ to 4 decimal places.

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:

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

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 $\{1, 2, \dots, n\}$ 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 Figure 1.

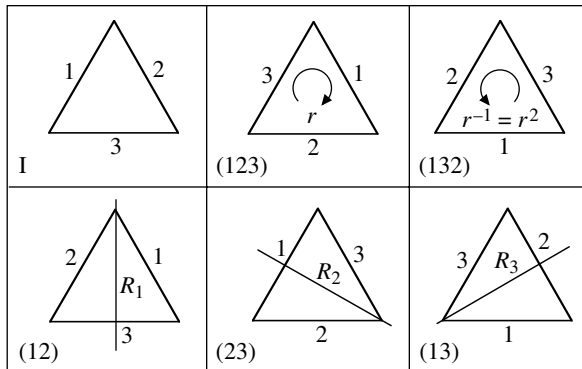


Figure 1. Symmetry group = S_3 .

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 in Table 1.

In 3 dimensions, we need to add one more kind of 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.

More information about the geometry of isometries in 3 dimensions 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 his or her own coat back?

If no one receives his or her 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 $1, 1^*, 2, 2^*, \dots, n, n^*$, 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 a 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 situation with 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

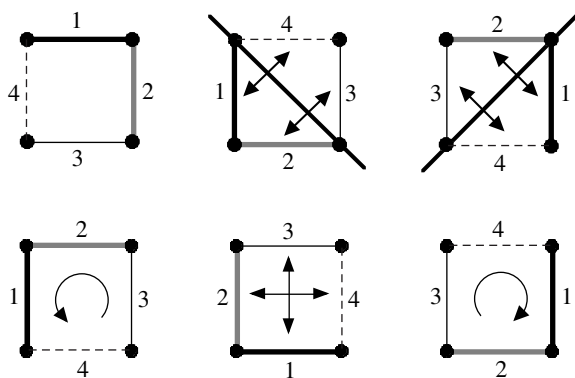


Figure 2. The 5 side-derangements of the square.

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 Section 5. For now, though, see if you can determine which isometries of the 3-cube are derangements. As a check, you should get the following:

- For the cube, there are 29 c-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 $\{1, 1^*, \dots, n, n^*\}$. 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 [11], although the interpretation in terms of c-derangements is new.

Theorem 1. *The number \hat{d}_n of c-derangements of the facets of Q_n is given by*

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

Proof. As with ordinary derangements, we count c-derangements via inclusion-exclusion. 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 count the number of ways to fix a specified set of k facets, we fix those facets (which also fixes the k opposite facets) and permute the remaining $n - k$ pairs of opposite facets in $2^{n-k} (n - k)!$ ways (the number of isometries of an $(n - k)$ -dimensional hypercube). Since there are $\binom{n}{k}$ ways to choose the specified k facets, inclusion-exclusion gives us the formula. ■

Note that a consequence of this formula is that $\hat{d}_0 = 1$. As before, 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

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

gives us the following:

In the couples coatcheck problem, the probability that no one receives his or her 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 $e^{-1/2} \approx 0.606531 \dots$ is accurate to 5 decimals. The associated 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.

There is another formulation we like that expresses \hat{d}_n in terms of ordinary derangements.

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

n	0	1	2	3
\hat{d}_n	1	1	5	29
$\frac{\hat{d}_n}{2^n n!}$	1	0.5	0.625	0.6041 ...
n	4	5	6	7
\hat{d}_n	233	2329	27,949	391,285
$\frac{\hat{d}_n}{2^n n!}$	0.606770 ...	0.606510 ...	0.606532 ...	0.606530 ...

Proposition 1. *The number of c-derangements of the facets of Q_n is*

$$\hat{d}_n = \sum_{k=0}^n \binom{n}{k} 2^k d_k. \quad (5)$$

Proof. Each c-derangement either sends a pair of opposite facets to another pair of opposite facets, or it fixes the pair (necessarily swapping the two facets in that pair). First choose k pairs of facets that are *not* swapped with their opposites. These k pairs can be deranged in d_k ways. For each pair that gets deranged, there are two ways to send it to its image pair. This gives $2^k d_k$ c-derangements; summing over all possible choices for selecting the k facets gives the formula. ■

A generalization of equation (5) appears in [12], 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 2. *For $n \geq 2$, \hat{d}_n satisfies:*

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

Proof. We consider two cases for any c-derangement of $\{1, 1^*, \dots, n, n^*\}$.

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 mapped to some other pair (k, k^*) . There are clearly $n - 1$ choices for the (k, k^*) pair, and 2 ways to map $(1, 1^*)$ to (k, k^*) . Suppose the pair (i, i^*) maps to $(1, 1^*)$, where i and k may or may not be equal. In either case, we can get a permutation of $2, 2^*, 3, 3^*, \dots, n, n^*$ by mapping (i, i^*) to (k, k^*) or (k^*, k) , depending on whether (i, i^*) mapped to $(1, 1^*)$ or $(1^*, 1)$ in the original c-derangement (and letting everything else map as in the original c-derangement).

We now have a permutation of $\{2, 2^*, 3, 3^*, \dots, n, n^*\}$. Is this permutation a c-derangement? Focusing on the possible images of k and k^* , we examine three possibilities.

1. If the permutation maps the pair (k, k^*) to some other pair, then it must be a c-derangement, and every c-derangement that moves the pair (k, k^*) arises in this way.
2. If the permutation swaps k and k^* , then it is still a c-derangement, and, as above, every c-derangement that swaps k and k^* arises in this way.
3. If the permutation fixes k (and, therefore, k^*), it is a c-derangement of the $n - 2$ pairs that remain after removing (k, k^*) .

The first two cases include all \hat{d}_{n-1} c-derangements of $n - 1$ pairs, and the final case (where k and k^* are fixed) includes all \hat{d}_{n-2} c-derangements of $n - 2$ pairs.

The recursion now follows. ■

Of course, we could prove the recursion (6) inductively by simply verifying it for either of the formulas (4) or (5), which we have already established. We believe such proofs are unsatisfying at some level, but make good exercises for students learning mathematical induction.

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, respectively. The direct isometries of a simplex correspond to even permutations of $\{1, 2, \dots, n\}$, 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).

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 $n \leq 7$.

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

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

A very casual glance at the last row of the table should suggest a very pretty theorem. This pattern is known; for example, you can find the sequences e_n and o_n in the OEIS [11]. A bijective proof using a conjugation argument can be found in [2], and the recent paper [8] offers two more proofs based on an analysis of excedances of permutations. The proof we give here is inductive and is included in the interest of keeping this paper as self-contained as possible.

Theorem 2. *Let e_n and o_n be the respective numbers of even and odd derangements of $\{1, 2, \dots, n\}$. 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 number of even derangements in which the transposition $(1r)$ appears for some $r > 1$ and e''_n denote the number of other even derangements; define o'_n and o''_n similarly. Then $e_n = e'_n + e''_n$ and $o_n = o'_n + o''_n$. Then we have the following recursive relations:

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

Then

$$\begin{aligned} e_n - o_n &= (e'_n + e''_n) - (o'_n + o''_n) \\ &= (n - 1)((o_{n-1} + o_{n-2}) - (e_{n-1} + e_{n-2})) \\ &= (n - 1)((o_{n-1} - e_{n-1}) + (o_{n-2} - e_{n-2})) \\ &= (n - 1)((-1)^{n-1}(n - 2) + (-1)^{n-2}(n - 3)) \quad (\text{by induction}) \\ &= (-1)^{n-1}(n - 1). \quad \blacksquare \end{aligned}$$

As an exercise, you can devise your own proof of Theorem 2 using determinants. First, let A be the $n \times n$ matrix with 0's on the main diagonal and 1's everywhere else (so $A = J - I$). Then you can use the permutation expansion of the determinant to show $|A| = e_n - o_n$. Finally, you can row reduce A to show $|A| = (-1)^{n-1}(n - 1)$.

Corollary 1. *Let e_n and o_n be the numbers of even and odd derangements, respectively. Then $e_n = (d_n + (-1)^{n-1}(n - 1))/2$ and $o_n = (d_n + (-1)^n(n - 1))/2$.*

We don't believe Theorem 2 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. Group theory for the cube. How can we determine whether an isometry of Q_n is direct or indirect? We know that a direct isometry is 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 better (in particular, more concise) way to represent an isometry. For readers who know more group theory, this recoding can be made precise by using the group of isometries of the hypercube, called the *hyperoctahedral* group (it's the same as the isometry group of the dual solid—the *hyperoctahedron* or the n -dimensional *cross-polytope*; see Chapter 7 of [6] for more information). 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 .

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 $\mathbf{0}$.
- Finally, use reflections normal to the coordinate axes to move $\mathbf{0}$ to some other vertex v . (This collection of reflections generates the normal subgroup \mathbb{Z}_2^n .)

We saw this procedure earlier—see 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 exactly two facets adjacent to a given vertex can be realized as a single reflection. Then the factor \mathbb{Z}_2^n is generated by the n orthogonal reflections normal to the n coordinate axes, and S_n is generated by reflections corresponding to transpositions. It's worth noting, however, that this analysis follows from the orbit-stabilizer theorem: A given vertex v of the n -cube has orbit of size 2^n —you can send any vertex to any other vertex—while the stabilizer of v is generated by all the reflections through that vertex, which gives S_n . More information about this action can be found in [7], for example.

Another way to understand the direct-indirect issue here is to use *signed permutation matrices*, i.e., permutation matrices in which each nonzero entry is ± 1 . Situate the n -cube so that all its vertices are located at the points $(\pm 1, \pm 1, \dots, \pm 1)$. 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 sends the facet corresponding to e_i to another facet $\pm e_j$.

This means that every isometry of the n -cube corresponds to a unique signed permutation matrix, and it's clear there are precisely $2^n \cdot n!$ such matrices. So, 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.

4.3. Counting direct and indirect c -derangements. 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 numbers 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, \dots, x_n) to its antipodal point $(-x_1, \dots, -x_n)$. 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. 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 3. *Let \hat{e}_n and \hat{o}_n denote the numbers of direct and indirect c -derangements of Q_n respectively. Then $\hat{e}_n - \hat{o}_n = (-1)^n$.*

Proof. We will construct a bijection between the direct and indirect c -derangements that are not central inversion. For a given c -derangement σ , find the smallest integer k so that the facet k is not swapped with its opposite facet. Then the map $\sigma \mapsto \sigma(k, k^*)$ gives the bijection between direct and indirect c -derangements (except for central inversion). Since central inversion is direct in even dimensions and indirect in odd dimensions, the result follows. ■

If you like, it's easy to reformulate the proof of this theorem using signed permutation matrices. Let A be a signed permutation matrix corresponding to a c -derangement that is not central inversion. Then A has at least 2 nonzero entries off the main diagonal, so we can find the smallest k with $A_{k,k} = 0$. Then multiplying column k of A by -1 gives the same bijection.

By the way, Theorem 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 2. *Let \hat{e}_n and \hat{o}_n denote the numbers of direct and indirect c -derangements of Q_n respectively. Then $\hat{e}_n = (\hat{d}_n + (-1)^n)/2$ and $\hat{o}_n = (\hat{d}_n + (-1)^{n+1})/2$.*

The sequences \hat{e}_n and \hat{o}_n appear to be new—when we began this work, we did not find them in the OEIS [11]. They now appear as sequences A161936 and A161937.

5. DERANGEMENT GEOMETRY IN DIMENSION 3. 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 general-

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

ize. 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 [6].

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*.

The tetrahedron has 24 symmetries corresponding to the $4!$ permutations of S_4 . Below, we classify these isometries. Before reading further, we highly recommend that you make your own list, either with a physical tetrahedron or, more of a challenge, in your head. The practice of the latter is great brain calisthenics.

- Direct isometries
 - The identity is clearly not a derangement.
 - The 8 rotations with axis through a vertex and the center of the opposite facet are not derangements.
 - The 3 180° rotations with axis through the centers of two opposite edges are derangements.
- Indirect isometries
 - The 6 reflections with mirror plane containing one edge of the tetrahedron are not derangements.
 - The 6 rotary reflections, pictured in Figure 3, are derangements.

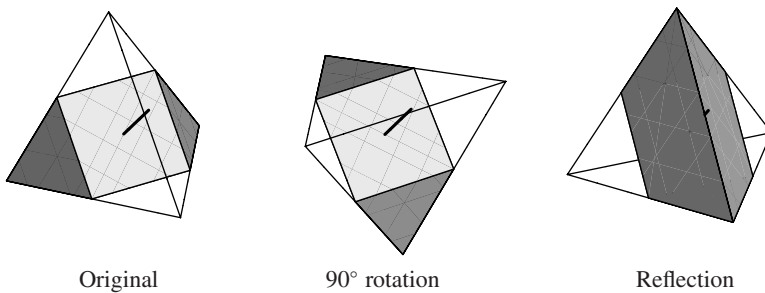


Figure 3. A rotary reflection in two steps: First rotate (the tetrahedron does not match up), then reflect.

It's worth investigating how the rotary reflections operate. The following step-by-step guide should help you create any of the 6 rotary reflections on your own (actual or virtual) 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 by itself is also not an isometry of the tetrahedron. However, from Figure 3, it's clear that the composition is indeed an isometry of the tetrahedron.

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 the 180° edge-rotations in the list of direct isometries. 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 $2^3 3! = 48$ isometries of a cube. We list them below, although you should try to come up with the list yourself first. Extra credit to those who find them all in their heads. We provide a figure for the rotary reflections, as they are the hardest to picture.

- Direct isometries
 - The identity is not a c-derangement.
 - The 8 rotations through pairs of opposite vertices are c-derangements.
 - The 6 rotations through centers of opposite edges are c-derangements.
 - The 9 rotations through centers of opposite faces are not c-derangements.
- Indirect isometries
 - None of the 9 reflections (3 reflecting opposite faces and 6 through opposite edges) are c-derangements.
 - The 15 rotary reflections are c-derangements. They are: central inversion (pictured in Figure 4a), 6 reducible ones through an axis through centers of opposite sides (pictured in Figure 4b), and 8 irreducible ones through an axis through two opposite vertices (pictured in Figure 4c). In Figure 4, opposite faces have the same pattern, but in different sizes.

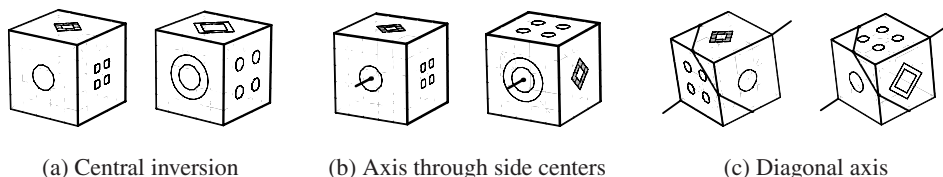


Figure 4. The 15 indirect face-derangements of the cube.

Note that 14 of the 29 c-derangements are direct, while 15 are indirect. The direct isometries preserve the orientation of the cube (so you could 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).

The indirect c-derangements are all rotary reflections. Central inversion always corresponds to a c-derangement (see Figure 4a), 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 4b, 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 4c, 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 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 5 breaks an irreducible rotary reflection down to help with visualization. Start with a hexagon that passes through each of the six faces of the cube. Instead of the direct isometry that rotates that hexagon through 120°, we rotate through 60° (not an isometry of the cube by itself) and then reflect.

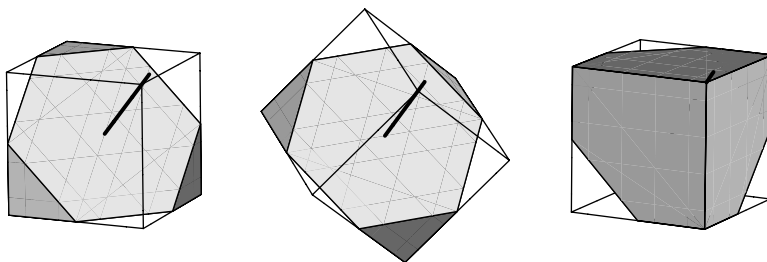


Figure 5. An irreducible rotary reflection of the cube.

There are two aspects of this kind of rotary reflection worth noting. First, it gives a 6-cycle on the faces of the cube. Second, the regular hexagon that passes through each of the 6 sides of the cube is well worth locating 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 3, we 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. Generalize other formulas for derangements to c-derangements. Here are two standard examples.
 - Ordinary derangements satisfy the recursion $d_n = nd_{n-1} + (-1)^n$. Show that the analogous recursion holds for c-derangements: $\hat{d}_n = 2n\hat{d}_{n-1} + (-1)^n$.
 - Rounding $n!/e$ to the nearest integer gives d_n . Show that rounding $2^n n!/\sqrt{e}$ to the nearest integer gives \hat{d}_n .
3. 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.

4. Study higher-dimensional solids. There are 6 regular solids in 4 dimensions: the 4-simplex, the hypercube, the hyperoctahedron, 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 coincide, since the vertex derangements for the 120-cell are the same as the 3-dimensional facet derangements for the 600-cell, etc.)
- For each class of derangements, count the direct and indirect isometries.

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 -simplex, the n -cube, and its dual, the n -dimensional hyperoctahedron. A generating function approach for the number of derangements of the k -dimensional faces of the n -cube is given in [4].

5. 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 [7].

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A Fifth Proof of an Inequality

We give another proof of the inequality in [1].

Theorem. *The sequence given by $u_n = (1 + 1/n)^{n+1/2}$ is decreasing, so greater than its limit, e .*

Proof. For $n \geq 1$, we have

$$\begin{aligned} \left(\frac{u_n}{u_{n+1}}\right)^2 &= \frac{\left(\frac{n+1}{n}\right)^{2n+1}}{\left(\frac{n+2}{n+1}\right)^{2n+3}} \\ &= \frac{(n+1)^{4n+4}}{n^{2n+1}(n+2)^{2n+3}} \\ &= \frac{n}{n+2} \left(\frac{n^2+2n+1}{n^2+2n}\right)^{2n+2} \\ &= \frac{n}{n+2} \left(1 + \frac{1}{n^2+2n}\right)^{2n+2} \\ &> \frac{n}{n+2} \left(1 + \frac{2n+2}{n^2+2n} + \frac{(2n+2)(2n+1)}{2(n^2+2n)^2} + \frac{(2n+2)(2n+1)(2n)}{6(n^2+2n)^3}\right) \\ &= \frac{3n^5 + 24n^4 + 72n^3 + 97n^2 + 51n + 8}{3n^5 + 24n^4 + 72n^3 + 96n^2 + 48n} \\ &> 1. \end{aligned}$$

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