Counting unlabelled nets of n-hypercubes

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1 Preliminaries

By Burnside's Lemma, the number of unlabelled nets of a hypercube of dimension n is

$$\frac{1}{|B_n|}\sum_{\mathrm{Cl}_{B_n}(g)\subseteq B_n}\#\mathrm{Cl}_G(g)\times\#\{\text{nets fixed by } g\}$$

where B_n is the hyperoctohedral group in n dimensions and we sum over conjugacy classes. $|B_n| = 2^n n!$

I'll write G_{2n} for the octohedral graph on $2n$ vertices, a net is then given by a spanning tree of this graph, with vertices labelled $(1, 2, \cdots, n, -1, \cdots, -n)$

[I have not proven that all such nets actually embed when unfurled into $n-1$-dimensional space; this seems likely but we'll not require it here.][1]

Labelling the faces $\{\pm 1, \cdots, \pm n\}$ the cycle type of some face (thinking of $B_n \subset S_{2n}$) might be conjugate in B_n to $(1\cdots k)$ (in which case we also have the cycle $(-1\cdots -k)$) or $(1\cdots k -1\cdots -k)$. Labelling the pair of cycles for the first option k and the second option $-k$ the conjugacy class of an element in B_n is then uniquely determined by a multisetC_g of things in $\{1,\cdots,n,-1,\cdots,-n\}$ whose absolute values add up to n. To get the cycle type of our element in S_{2n} we have 2 copies of i for every $i > 0$ in C_g and a $2i$ for every $-i$. Write the number of copies of a in C_g as c_a

We can calculate $|\mathrm{Cl}_{B_n}(g)| = |B_n|/|C_{B_n}[g]|$ by calculating the size of the centralizer of g. There are $2k$ group elements on B_k which commute with $(12\cdots k)(-1-2\cdots -k)$ or $(1\cdots k -1\cdots -k)$ (i.e powers of these elements times perhaps inversion about the origin in the first case); these elements for each cycle in g together with $c_a!$ permutations of the cycles of type a generate the centralizer. We have

$$|C_G[g]| = \prod_a c_a!(2|a|)^{c_a}$$

Any automorphism of a tree of must fix either at least one vertex (we'll choose one WLOG) or fix an edge (and we can stipulate the edge is reversed and is unique). The shortest proof of this is probably to use Lefschetz' fixed point theorem but if I can I can see if I can find an explanation that requires less technical machinery.

We'll write $C_{i,a}$ for the ith cycle of length a in the action of g on the vertices of the graph G_{2n}.

[1] For any cycle in $\mathbb{Z}^{n-1}$ and for any direction (wlog left-right) the cycle's edges go along consider the exit and entry point at a connected component of the leftmost edge of the cycle. The 2 $n-1$-cubes just to the right of these entry and exit edges roll up into the same face of the n hypercube, so the net of the hypercube cannot give rise to this cycle. We can also use this to deduce the adjacency graph of the $n-1$-cubes is a tree

Consider the cycles $C_{i_k,a_k}, C_{i_{k-1},a_{k-1}} \cdots C_{1,a_0}$ and $a_0 \in \{1,2\}$ we visit when we take the unique path from some element in the graph to either our chosen fixed vertex or the closest endpoint of the fixed edge. We generate the same set of cycles no matter which element of C_{i_k,a_k} we start at, and any final segment of this path must also be a unique path of this kind, so we can only visit each cycle once.

Labelling the vertices in C_{i_k,a_k} $(v_1, \cdots, v_{a_k})$ and those in $C_{i_{k-1},a_{k-1}}$ $(w_1, \cdots, w_{a_{k-1}})$ any v must connect to a unique w in the tree, and v_t connects to w_s iff v_{t+1} connects to V_{s+1}. So a_{k-1} must divide a_k. If C_{i_k,a_k} and $C_{i_{k-1},a_{k-1}}$ do not share the same axes every w is connected to every v there are a_{k-1} ways to arrange this, if they are opposie to each other v_i cannot connect to $-v_i$ but all other $a_{k-1} - 1$ possibilities can be arranged.

For any possible rooted tree with vertices labelled by the $C_{i,a}$ with C_{0,a_0} as the root satisfying these divisibility criteria and for any arrangement among the a or $a - 1$ for each ourward edge from $C_{a,i}$ to $C_{b,j}$ we do in fact get a tree that is preserved by g. In the case $a_0 = 2$ we require the two vertices of C_{0,a_0} to be connected by an edge – this cycle must come from a 2 and not a -1 in C_g.

(I'm not sure whether there's a usual convention here but here a spanning tree means we can reach everywhere outward from the root.)

2 Algorithm

We now are ready to present the following algorithm for computing the number of nets of an n-hypercube. Write the number of copies of a in C_g as c_a

- Iterate over all the C_g:
- Calculate the following function $\mathrm{Tr}(g)$: the number of trees preserved by the action of g on G_{2n}.
  - g can only fix a vertex if $c_1 > 0$ if this is the case we then construct a multi-directed graph H_g with vertices labelled by the $C_{i,a}$ with no loops on the cycles of g in S_{2n} with
    - No edges from $C_{i,a}$ to $C_{j,b}$ if a does not divide b.
    - $a - 1$ edges from $C_{i,a}$ to $C_{j,a}$ if these cycles happen to be opposite to each other
    - a edges from $C_{i,a}$ to $C_{j,b}$ otherwise.

    We then let $\mathrm{Tr}(g)$ be the number of spanning trees with some 1-cycle as the root, which we can enumerate using e.g Kirchoff's Matrix theorem. In the case where $c_1 = 1$ and we have two 1-cycles it happens that $\mathrm{Tr}(g) = 0$; it is impossible to connect whichever vertex is the root to the other.
  - g can only fix an edge if C_g has at $c_2 > 1$ copies of 2 (and no copy of 1). We construct exactly the same graph and enumerate the number of spanning trees with some 2-cycle as the root. Unlike in the first case different choices of the 2-cycles give rise to different trees, so $\mathrm{Tr}(g) = 2c_2$ times this number of spanning trees. No such spanning tree exists if we have an odd cycle, ie if $c_{2i+1} \neq 0$ for some $i \geq 0$.
  - In all other cases no tree preserved by g exists and $\mathrm{Tr}(g) = 0$

- Calculate the number of conjugacy classes

$$|\mathrm{Cl}_{B_n}(g)| = \frac{n!2^n}{\prod_a c_a!(2|a|)^{c_a}}$$

- Sum up

$$\frac{1}{|B_n|} \sum_{Cl_{B_n}(g) \subseteq B_n} Tr(g) * |\mathrm{Cl}_{B_n}(g)|$$

3 A somewhat faster way to compute $Tr(g)$

We notice that our spanning tree T for H_g must also be a spanning tree when restricted to the subgraph $H_g[C_{*,<a}]$ on all the vertices corresponding to cycles of size less than a for any $a > a_0$. Further, sufficient and necessary conditions for $T[C_{*,<a+1}]$ to be a tree are

- $T[C_{*,<a}]$ is a spanning tree
- $T[C_{*,a}]$is a forest
- Every connected component of $T[C_{*,a}]$connects exactly once to some $C_{*,b}$ with $b < a, b|a$. Noticably this is not affected by $T[C_{*,<a}]$

We can therefore generate trees in $H_g[C_{*,<a}]$ and compute Tr(g) as follows: First, we generate $T[C_{*,a}]$. For the case $a_0 = 1$. By Kirchoffs matrix tree the number of trees we can choose from is the determinant of the $2c_1 - 1 \times 2c_1 - 1$ matrix

$$\begin{pmatrix} 2c_1-2 & 0 & -1 & \cdots & -1 & -1 \\ 0 & 2c_1-2 & -1 & & -1 & -1 \\ -1 & -1 & 2c_1-2 & & -1 & -1 \\ \vdots & & & \ddots & & \vdots \\ -1 & -1 & -1 & \cdots & 2c_1-2 & -1 \\ -1 & -1 & -1 & \cdots & -1 & 2c_1-2 \end{pmatrix}$$

Our eigenvalues are $c_1 - 1$ copies of $2c_1 - 2$ from vectors of the form $e_{2i-1} - e_{2i}$, $c_1 - 2$ copies of $2c_1$ from vectors of the form $e_{2i-1} + e_{2i} - e_{2i+1} - e_{2i+1}$. Our matrix acts on the vectors orthogonal to this of $e_1 + \cdots + e_{2c_1-2}$ and e_{2c_2-1} by

$$\begin{pmatrix} 2 & -2c_1+2 \\ -1 & 2c_1-2 \end{pmatrix}$$

which has determinant $(c_1 - 1)$. So the determinant we want is

$$(2c_1 - 2)^{c_1}(2c_1)^{c_1-2}$$

For the case $a_0 = 2$ the number of trees we can choose from is the determinant of the $v - 1 = 2c_2 + c_1 - 1 \times v - 1$ matrix M with

$$M_{ij} = \begin{cases} 2v-3 : i = j \leq 2c_2 - 1 \\ 2v-2 : i = j > 2c_2 - 1 \\ -1 : i = 2k-1, j = 2k \text{ or } i = 2k, j = 2k-1 \text{ with } k \leq c_2 - 1 \\ -2 : \text{else} \end{cases}$$

which we can compute by a similar method has determinant

$$2^{v-c_2-1}v^{v-c_2-2}(2v-1)^{c_2}$$

Now we consider how to add $H_g[C_{*,a}]$ to an already existing tree $T[C_{*,<a}]$. $H_g[C_a]$ has $2c_a + c_{-a/2}$ vertices (where we set $c_{-a/2} = 0$ if $-a/2$ is non-integer).

There are

$$p_a = \sum_{b<a;b|a} 2bc_b + bc_{-b/2}$$

possible vertices we can connect each of our connected components in our forest to.

This is equivalent to the problem of finding rooted spanning trees of a graph on $V[H_g[C_a]] \cup \{W\}$ from W, where there are p_a connections from W to every vertex in $H_g[C_a]$. Again, to enumerate the ways of doing this, using Kirchoff's matrix tree theorem, we want to find the determinant of the $v = 2c_a + c_{-a/2} \times v$ matrix M

$$M_{ij} = \begin{cases} a(v-1) - 1 + p_a : i = j \leq 2c_a \\ a(v-a) + p_a : i = j > 2c_a \\ -a+1 : i = 2k-1, j = 2k \text{ or } i = 2k, j = 2k-1 \text{ with } k \leq c_a \\ -a : \text{else} \end{cases}$$

which is

$$p_a(va + p_a)^{v-c_a-1}(va + p_a - 1)^{c_a}$$

.

So, after computing

$$p_a = \sum_{b<a;b|a} 2bc_b + bc_{-b/2},$$

we can calculate $\mathrm{Tr}(g)$

If $c_1 \geq 2$

$$\begin{aligned}\mathrm{Tr}(g) = \\ &(2c_1-2)^{c_1}(2c_1)^{c_1-2} \\ &\times \prod_{a>1} p_a(a(2c_a + c_{-a/2}) + p_a)^{c_{-a/2}+c_a-1}(a(2c_a + c_{-a/2}) + p_a - 1)^{c_a}\end{aligned}$$

If $c_1 = 0, c_2 \neq 0$ and $c_{2i+1} = 0$ for $i \geq 0$ (multiplying in the $2c_2$ term):

$$\begin{aligned}\mathrm{Tr}(g) = \\ &2^{c_2+c_{-1}}c_2(2c_2 + c_{-1})^{c_2+c_{-1}-2}(4c_2 + 2c_{-1} - 1)^{c_2} \\ &\times \prod_{a>1} p_a(a(2c_a + c_{-a/2}) + p_a)^{c_a+c_{-a/2}-1}(a(2c_a + c_{-a/2}) + p_a - 1)^{c_a}\end{aligned}$$

and in all other cases

$$\mathrm{Tr}(g) = 0$$

4 Asymptotics

I believe that the number of nets asymptotes to

$$\frac{c\mathrm{Tr}(e)}{|B_n|} = \frac{c(2n)^{n-2}(2n-2)^n}{(2^n n!)} \sim \frac{c}{\sqrt{\pi}} e^{n-1}(2n)^{n-\frac{5}{2}}$$

for

$$c = e^{\frac{1}{2}(e^{-2}+e^{-4})} \approx 1.07985$$

I do know the following, which is very suggestive:

For any finite multiset of elements drawn from $\mathbb{Z}^- \cup \mathbb{Z}_{\geq 2}$, we have a conjugacy class $Cl_{B_n}[g_n]$ for all large enough B_n where we preserve all other faces of the cube.

Then

$$\lim_{n\to\infty} \frac{\mathrm{Tr}(g_n)\mathrm{Cl}_{B_n}(g_n)}{\mathrm{Tr}(e)} = \frac{e^{-2a_{-1}-4a_2}}{2^{a_{-1}+a_2}a_{-1}!a_2!}$$

if $a_i = 0$ for all $i \neq 1, -1, 2$, and

$$\lim_{n\to\infty} \frac{\mathrm{Tr}(g_n)\mathrm{Cl}_{B_n}(g_n)}{\mathrm{Tr}(e)} = 0$$

otherwise.

5 Implementation/Results

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 n 12-core-sec count

1 0.245348930 0

2 0.247266054 1

3 0.239933729 11

4 0.204809188 261

5 0.215048551 9694

6 0.218962192 502110

7 0.231381177 33064966

8 0.244138002 2642657228

9 0.248214006 248639631948

10 0.255265951 26941775019280

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